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## *TECHNICAL ABSTRACTS*

### TWO-DIMENSIONAL PREDICTIONS OF POLLUTANT EMISSION AND HEAT TRANSFER CHARACTERISTICS IN POROUS BURNERS: A VALIDATION STUDY

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Several mathematical models with varying degrees of sophistication have been applied to study combustion and heat transfer in inert porous media. The majority of such models focus on one-dimensional geometries and should not be applied to the study of complex, real porous burners.

In this study, a two-dimensional numerical model was developed to predict heat transfer and premixed combustion inside a porous burner. Separate energy equations for the solid and gas phase mechanism was described by the skeletal mechanism of Glarborg et al. (1992) that consists of 77 reactions and 26 species. The two-dimensional discrete ordinates method was used to describe the radiative transfer equation and the porous media was assumed to emit, absorb and isotropically scatter radiation. The finite difference/control volume approach was used and the SIMPLE algorithm applied. Since the mass fraction conservation equations are stiff, an operator splitting method was used to solve them.

Predicted gas and solid centerline temperatures were compared with available experimental data for a porous burner with integrated heat exchanger prototype developed for household applications. The results show satisfactory agreement between the predictions and the experimental data. Predicted CO and $NO_x$ emissions were also compared with experimental data. Good predictions of CO and overestimation of $NO_x$ were obtained. Radiation was found to be very important in the modeling of the porous burner and an accurate radiative model and correct radiative properties essential for the correct prediction of the overall performance of a porous media combustor. Unfortunately, a good database for the radiative properties of some commonly used porous media is lacking, requiring sensitivity studies. The present multidimensional model proved to give interesting engineering solutions for the fluid flow, heat transfer, pollutant emissions and combustion occurring in inert porous media. To our knowledge, it is the first time that an attempt to predict the two-dimensional fields of these quantities for a porous burner prototype is made. Since nowadays it is impossible to obtain three-dimensional flow predictions inside each pore, additional work is required in order to gain a better understanding of the combustion inside porous inert media, such as the inclusion of the reactions on the solid surfaces of the solid matrix.

## CHEMICAL STRUCTURES OF METHANE-AIR FILTRATION COMBUSTION WAVES FOR FUEL-LEAN AND FUEL-RICH CONDITIONS

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Filtration combustion of gases within inert porous media has been extensively studied during the last decade. Particular attention was given to the low-velocity regime of filtration combustion, characterized by low degree of thermal non-equilibrium between solid and gas phases. In this regime, the strong interfacial heat exchange allows so-called superadiabatic combustion of gaseous mixtures with very low adiabatic combustion temperatures. Earlier work focused exclusively on lean combustion, studying the enhancement of the maximum temperature under these conditions. Unfortunately, there is an absence of work covering the broader range of equivalence ratios from lean to rich mixtures.

In the present work, results of a comparative study of filtration combustion from lean to rich mixtures are presented with the emphasis on the chemistry of the combustion waves. Temperature, velocity and chemical products of the combustion waves are studied experimentally in the range of equivalence ratios from 0.2 to 2.5. Downstream (superadiabatic) wave propagation is observed for ultra-lean ($\varphi \leq 0.45$) an ultra-rich ($\varphi \geq 1.6$) mixtures. Upstream (underadiabatic) propagation corresponds to the range of equivalence ratios from 0.45 to 1.6. It is found, that with the equal heat content, rich mixtures have essentially higher combustion temperatures than corresponding lean mixtures.

Stable superadiabatic combustion of ultra-rich mixtures is observed experimentally for the region of equivalence ratios above 1.6. In this region, complete combustion could not be achieved due to the low oxygen content in the mixture. This results in formation of partial oxidation products such as $H_2$, CO and $C_2$ hydrocarbons. These products became dominant for equivalence ratios above 2, where up to 60% of methane is converted to CO and $H_2$.

Predictions of a numerical model based on a one-temperature approximation and multistep gas phase combustion mechanism, is in good agreement with experimental data, including combustion temperatures and combustion products. Reaction pathway and sensitivity analysis shows significant changes in the combustion mechanism from ultra-lean to ultra-rich conditions. $C_1$-mechanism, dominant for ultra-lean conditions, is suppressed by $C_2$-mechanism for ultra-rich mixtures.

Kinetic modeling revealed that the ultra-rich superadiabatic combustion wave is composed of an exothermic reaction zone followed by an endothermic one. In the exothermic wave, partial oxidation of methane takes place with formation of hydrogen, carbon monoxide and water. Subsequently, the reaction of "steam reforming" occurs in the endothermic region where unburned methane is reformed by water with production of additional hydrogen and carbon monoxide.

## COMBUSTION OF SOLID WASTE IN A PULSE INCINERATOR

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Increasingly strict regulations on the disposal of waste on board ships has generated new interest in compact, high efficiency, low pollution incinerators. It is the purpose of this study to investigate whether a pulse incinerator could meet these criteria.

The effect of acoustic oscillations on the combustion of simulated solid wastes in a pulse incinerator were studied. The incinerator consists of a rectangular metal box with inside dimensions 108x20x12 cm. Air enters through a 2.5 cm diameter pipe and exhaust gases leave through a 5.0 cm diameter pipe. Two 13x13 cm fused quartz windows located in opposite side

panels near the sample location provide optical access to the combustion region. An igniter, fitted to the bottom of the incinerator, provides a repeatable ignition process at the beginning of each test. Acoustic oscillations inside the cavity are driven by two 100 W Atlas siren drivers through a closed loop control system. A flush mounted, Kistler piezoelectric pressure transducer, located next to the solid waste surrogate, monitors the pressure oscillations during combustion. Gas samples are extracted from the exhaust line and passed through a sampling line into Beckman $CO_2$, CO and $NO_x$ analyzers. The $CO_2$ trace was used to characterize the burning rate and combustion time because $CO_2$ is the primary combustion product. When the surrogate waste burns with a visible flame prior to smoldering (cardboard samples), flaming and smoldering combustion times were recorded separately. Total amounts of $CO_2$, CO and $NO_x$ emitted are calculated by integrating $CO_2$, CO and $NO_x$ traces.

Corrugated cardboard and charcoal were chosen as waste surrogates because of their different combustion characteristics. Cardboard burns with a luminous, gas phase flame followed by a solid phase, smoldering combustion. Charcoal, on the other hand, burns mainly by smoldering. For both fuels, it was shown that pulsations greatly increase combustion rates. This enhancement was of the order of 65% whether the sample was smoldering or burning with a flame. While the increase in burning rate in the presence of a flame appears to have been caused by increased pyrolysis of the fuel, the large smoldering rate enhancement seems to be due to an increase in the rate of diffusion of air to and combustion products from the burning surface. The pulsations also enhanced the rates at which CO and $NO_x$ are produced. However, because the increased burning rates resulted in shortened combustion times, the total amount of CO and $NO_x$ emitted was not significantly affected by the pulsations.

In order to determine to what extent the observed acoustic enhancement of the combustion process would persist in more turbulent flows found in practical incinerators, the Reynolds number of the flow through the incinerator was varied between 4,700 and 47,000. In the absence of pulsations, increasing the Reynolds number resulted in increased burning rates. However, when combustion occurred in the presence of high amplitude acoustic oscillations (158 dB), the combustion time was observed to be independent of the Reynolds number. At this dB level the charcoals burned twice as fast as in steady flow at the highest Reynolds number (Re=47,000). The total CO and $NO_x$ emissions were approximately the same regardless of Reynolds number and the presence or absence of pulsations.

In summary, the above results suggest that pulse incinerators will be able to handle significantly increased waste throughputs without increased pollutant emissions.

## CO-FIRING HIGH SULFUR COAL WITH REFUSE DERIVED FUELS

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The ability to capture $SO_2$ and halogens is one of the most important advantages of fluidized bed combustion (FBC). This project was designed to evaluate the combustion performance of and emissions from a fluidized bed combustor during the co-firing of mixtures of high sulfur and high chlorine coals or municipal solid waste (MSW). The experimental investigation was carried out on a bench scale laboratory AFBC system with the 0.3 m internal diameter and 4.5 m effective height at Western Kentucky University. During experiments, the PVC was mixed with coal in different weight percentages, and the mixture was fed into the FB combustor by screw feeder. The Ca/S mole rate was kept constant at approximately 3. The experimental results indicated that chloride addition dramatically decreases the $SO_2$ concentration in flue gas. At the same time, the sulfur content increases in both the fly ash and bed ash.

The effect of sulfur dioxide on the formation of molecular chlorine during combustion processes was also examined in this study. Sulfur dioxide has been proven to be an effective inhibitor for the formation of molecular chlorine through the reaction:

$$Cl_2 + SO_2 + H_2O \rightarrow 2HCl + SO_3$$

and subsequently, the production of chlorinated organic. The co-firing of MSW and high sulfur coal seems to be a promising method to reuse MSW in the future.

## OXIDATION RATES OF SOOT PARTICULATES WITH OH AND NO UP TO VERY HIGH TEMPERATURES IN SHOCK WAVES

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The oxidation rates of soot particulate aerosols were studied behind reflected shock waves between 1150 and 3000 K and pressures 3-15 bar in dilute $H_2/O_2$ mixtures in argon. The rates found in the region 1150-1800 K obeyed Arrhenius kinetics and were fast compared to those in $O_2$/argon or NO/argon. Above 1800 K the rate showed non-Arrhenius behavior. The rates went through a maximum in the region above 1800 K before decreasing but then showed a further increase at still higher temperatures. The rates exhibited first order dependence on $H_2$ but were independent of $O_2$ below about 1800 K. This is different to the order of 0.5 obtained for the $O_2$ alone. It is suggested that the hydroxyl radical is the most reactive species in these mixtures with a surface collision probability of reaction $\alpha \approx 0.25(\pm 0.1)$ between 1150-1800 K. Above this temperature range the apparent value of $\alpha$ decreased, due to the apparent decrease in rate. The reasons for this are not clear and are discussed in the paper.

The rate of disappearance of soot in nitric oxide/argon mixtures at pressures of 5-7 bar was measured between 2000-3300 K. These rates gave linear Arrhenius plots and were found to be first order in NO. The rate of reaction of soot with NO can be represented by the equation:

$$\alpha_{NO} = 4.08 \exp(-135800\ J/RT)$$

where $\alpha$ = the surface collision probability.

With argon only present (pressures 11-13 bar) and at temperatures above 2900 K, the soot particulates were found to disappear slowly. Between 3200-3800 K this rate became significant and the process had an activation energy of 215 kJ/mol which is much less than the enthalpy of vaporization of carbon.

At temperatures above 2500 K the temperature dependence and rates of reaction of soot in the presence of $O_2$, $O_2/H_2$, NO were not dissimilar to those in argon. The effect can be explained using the results found by other workers investigating the laser heating of soot in flames by LII (laser induced incandescence) which produced a surface temperature of around 4000 K similar to the temperatures used in some of this work. LII heating produced the formation of $C_2$ and $C_3$ species. It is suggested that similar reactions can also occur in very high temperature thermally heated soot particulates in this work.

## EFFECT OF LOWER STATE ROTATIONAL ENERGY TRANSFER UPON TEMPERATURE MEASUREMENTS MADE WITH LASER INDUCED FLUORESCENCE

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Laser induced fluorescence (LIF) is often used to deduce gas temperatures from the relative populations of two rotational states. As a realistic example, we model the atmospheric combustion of methane with air, with products that are 2000 K. We calculate the ratio of fluorescence intensities that would be induced by doubled dye-laser light near 283 nm, by means of the $A \leftarrow X$, $1 \leftarrow 0$, $P_1(7)$ and $Q_2(11)$ transitions in OH. Here we show that the ratio of LIF signals from those transitions, and thus the deduced temperature, is sensitive to laser intensity. We emphasize the competition between laser-pumping of molecules out of the lower rotational state and of rotational

energy transfer (RET) collisions into that state. RET occurs in both the X- and A-states. Further, electronic (A→X) quenching occurs, usually into many vibrational states. Even for an idealized situation, with the same quenching rate for both A-state species, and without RET collisions in the A-state, the deduced temperature can vary by factors of two or three. The laser spectral intensity dependence of the fluorescence ratio can also depend heavily upon the value of the RET coefficients within the X-state. RET reduces the sensitivity of the observed signal to the laser spectral intensity. However the conversion of a measured fluorescence ratio to temperature is particularly difficult, because RET rates and quenching rates can be a function of local conditions and of the rotational state being populated.

While RET leads to much higher signals than would otherwise occur, these signals are difficult to interpret. They are dependent on location and on state-sensitive rate constants. Calibration can be done only for laser pumping that is sufficiently small that RET can maintain the original population of state 1. An alternative solution is to reduce the laser pulse length so that only a few molecules can flow into the ground state via RET during the time the laser is on.

## ROTATIONAL COHERENT ANTI-STOKES RAMAN SPECTROSCOPY FOR TEMPERATURE AND OXYGEN CONCENTRATION MEASUREMENTS IN PRACTICAL COMBUSTION DEVICES

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Coherent anti-Stokes Raman Spectroscopy (CARS) is a laser-based diagnostic technique which is used for non-intrusive temperature measurements in combustion processes. This poster concerns a variant of CARS called dual-broadband rotational coherent anti-Stokes Raman spectroscopy (DB-RCARS). DB-RCARS can be used for temperature and relative oxygen concentration measurements. The best accuracy of the technique is achieved in the temperature range up to 1500 K at pressures from atmospheric to a few MPa.

In DB-RCARS, three laser beams are focused to a common intersection point from which a signal is generated if suitable molecular resonances are available. The signal is generated as a laserlike beam. The spectrally resolved signal is analyzed by fitting its shape to a library of theoretically calculated spectra. Temperature evaluation is normally made from nitrogen spectra since nitrogen is inert and high concentrations of nitrogen are present in air-fed combustion.

In this poster some work on DB-RCARS for practical applications are described; 1) cycle-resolved temperature measurements in a spark ignition engine for knock studies, 2) measurements of temperature and relative oxygen concentrations after a catalytic combustor, and 3) a method for spectral discrimination of stray light, which is of special importance in practical applications.

The phenomenon of knock in spark ignition engines is studied in a project where the sub-projects are: evaluation of knock detection methods, modeling of flow and flame propagation, modeling of chemical kinetics, thermal analysis of heat transfer, and our sub-project on laser diagnostic temperature measurements using DB-RCARS. Cycle-resolved temperature measurements were performed in the unburned fuel/air mixture ahead of the propagating flame front at pressure below 2 MPa and temperatures below 1000 K. This is a range of conditions where the pure rotational CARS technique both has a high accuracy and a high precision. Measurements were performed at different crank angle degrees in the engine cycle, at different distances from the cylinder wall, and for different fuel mixtures.

In a project with the purpose to develop ceramic components for a gas turbine, DB-RCARS measurements were performed after a catalytic combustor section. Profiles of temperature and relative oxygen concentrations were measured across the section for four different running conditions. All measurements were performed remotely, meaning that the focusing and

recollimating lens in the setup were translated up to 10 cm during the measurements. High temperatures and low relative oxygen concentrations indicated a high efficiency at the central axis, and lower efficiency close to the wall. Also, emission measurements using conventional methods were performed after the catalytic combustion section.

In practical measurements using dual-broadband rotational CARS the major experimental problem is stray light from one of the primary laser beams. This radiation may interfere with the registered CARS spectrum at the detector. An atomic filter consisting of a sodium-seeded flame is presented as a solution to this problem.

### CARS TEMPERATURE MEASUREMENTS IN 1-D AND 2-D LAMINAR FLAMES

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Numerical chemical reaction models are used to accurately model for example industrial or household furnaces. To validate these models quantitative information on flame temperatures with a high spatial resolution is required using a measurement technique that does not perturb the flame. This was accomplished using broadband vibrational coherent anti-Stokes Raman spectroscopy (CARS). CARS temperature data were collected at a high spatial resolution and close to high temperature gradients for a set of 1-D and 2-D flames. Due to the geometrical properties of the flames the experiment could be aligned in such a way that the temperature gradients were perpendicular to the direction of the laser beams. We have investigated and mastered problems related to detection (using a high dynamical range back-illuminated CCD camera) and laser instability (shot-to-shot fluctuations and long-term spectral shift of the Stokes laser profile and, in the flame, beam steering). Uncertainties in the CARS fitting code (the non-resonant susceptibility, non-resonant background, detector background and instrumental slit width) and interfering laser-induced processes, such as stimulated Raman pumping, were also analyzed.

In this poster we will present accurate temperature measurements, along with calculated profiles, obtained for adiabatic flat flames and a 2-D V-flame. The V-flame, also known as the inverted flame, burns on a double slit burner. The burner is used to investigate the stabilization of laminar premixed flames. The stabilization point of the V-flame is not surrounded by air, but instead by the fuel/air mixture flowing out of the slits. Consequently, the surrounding atmosphere does not affect the stabilization of a V-flame, as is the case in the conventional Bunsen flame. These flames are therefore well suited to study blow-off mechanisms of Bunsen-type flames.

A series of measurements and calculations were also performed in a single slit burner. This burner is an idealized two-dimensional form of the well-know Bunsen burner. Modeling of this flame is done with detailed chemistry. To define boundary conditions in the numerical model the 2-D Bunsen flame was confined between two plates set at a fixed temperature.

### METHANE IGNITION PROMOTED BY $NO_x$

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Small amounts of nitrogen oxides have been shown to promote the oxidation of low concentrations (usually the order of hundreds of parts per million) of fuels at temperatures between 500 and 1000 K. The question as to the extent to which this effect may be significant

at higher fuel concentrations has not been addressed in any detail, despite the potential importance of this phenomenon to ignition such as autoignition, in engines, or in gassy mine environments where $NO_x$, fuel (mostly $CH_4$), and oxygen coexist.

In this work, we describe experimental and modeling studies of the effect of NO and $NO_2$ (0 to 400 ppm) on the ignition of methane (up to 2.5%) in air. The experiments are carried out in a flow reactor at atmospheric pressure and at temperatures from 820-920 K, with a residence time of the order of 2 seconds. Under the conditions studied, and in the absence of $NO_x$, no ignition of $CH_4$ is observed at temperatures below 900 K. However, when $NO_x$ is present as either NO or $NO_2$, there is a substantial reduction in the ignition temperature, to 870 K with 5 ppm $NO_x$, and to 820 K with 400 ppm $NO_x$. The presence of $NO_x$ promotes $CH_4$ consumption even in the absence of an ignition.

The high concentrations of $CH_4$ employed in this work are capable of giving rise to a substantial product temperature rise which cannot be modeled accurately for the tubular flow reactor. However, a model validated previously for the low-temperature ignition of low concentrations of $CH_4$ in the presence of $NO_x$ describes the results for $CH_4$, CO, $CO_2$ and $C_2$-species reasonably well under conditions where less than 20% conversion of $CH_4$ occurs, when the mixture is expected to be nearly isothermal.

The chief mechanism of promotion of the oxidation of $CH_4$ is the same as previously proposed, namely that NO converts the chain terminating methylperoxy radical into reactive methoxy:

$$CH_3O_2 + NO \rightarrow CH_3O + NO_2$$

These results demonstrate the importance of the $NO_x$-promoted oxidation of reasonably high concentrations of $CH_4$ at low temperatures, and the possibility of premature (low-temperature) ignition as a result of this effect. They also confirm the validity of the model developed previously.

## MEASUREMENT OF LOCAL FLAME-FRONT STRUCTURE IN TURBULENT PREMIXED FLAME

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LIF techniques have been improved to be able to investigate the flame front structure, while the time-series measurement of the flame-front has been obtained in order to understand the detail of flame-front structure and flame propagating speed.

Local chemiluminescence measurements of OH, CH and $C_2$ radicals were carried out in turbulent premixed methane flame to make clear the details of flame-front structures and chemical reactions in the reaction zone. For this measurement, specially designed Cassegrain Optics were developed, which have a high spatial resolution as small as an LDV measurement volume. Furthermore, to achieve a high temporal resolution, each chemiluminescence was detected by a photomultiplier tube at a sampling rate of 250 kHz.

Simultaneous measurements of these three radicals and velocity by LDV were performed to obtain flame-front structure, flame propagating speed and flame thickness. Local Damkoler number was measured directly at the flame-front and its fine scale demonstrated.

The probability density function (PDF) of OH emissions showed bi-modal peaks across the flame-front location corresponding to wrinkled laminar flame or flamelet region. The first peak of the OH PDF corresponded to the high temperature region outside of the flame cone and the secondary peak was associated with chemical reaction at the primary reaction zone. Time series signals of local OH, CH and $C_2$ emission intensities in wrinkled laminar flame region showed irregular peaks which, however, correlate in the three chemiluminescence signals. These results indicated strong linkage between OH-CH-$C_2$ reactions at wrinkled laminar flame-front. The flame-front thickness measured by CH and $C_2$ emissions were 0.1 and

0.3 mm, while being about 1.0 mm for OH. Furthermore, local reaction rate and local mixture strength at the turbulent flame-front are examined from local CH and $C_2$ emission intensities in comparison with measured databases of these emissions in laminar premixed flame.
A new optical diagnostics method to examine local flame-front structure and flame chemistry by means of local chemiluminescence measurements has been proposed and its performance proven.

QUANTITATIVE HYDROXYL TIME-SERIES MEASUREMENTS IN TURBULENT NON-PREMIXED FLAMES
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During the past two years, we have presented measurements of both CH and OH fluorescence time series via picosecond time-resolved laser induced fluorescence (PITLIF). However, these measurements lacked corrections for variations in the quenching rate coefficients. A rapid, gated photon-counting system, termed LIFTIME, has been built to allow on-the-fly quenching corrections to each point of a fluorescence time series. This photon-counting system divides the fluorescence decay into three equal temporal partitions and integrates the photon count within each of these areas. These three counts are then used to compute the lifetime, the peak amplitude of the fluorescence decay, and the flame emission background. The measured lifetime can then be used to correct the fluorescence time series point by point. Alternatively, the decay amplitude can be directly interpreted as concentration, as will be shown in the present work. Following this quenching correction, the time series are calibrated against well-characterized premixed flames. The result of the combination of PITLIF and LIFTIME is a system capable of quantitative time-series measurements of naturally occurring minor-species scalar fluctuations that can be used to develop or test combustion models. For example, the data can be used along with an assumed power spectral density (PSD), laminar-flamelet analysis to investigate the interactions between turbulence and chemical reaction.
The present work details the photon-counting system design and presents results of lifetime and concentration measurements in a series of laminar flames. These measurements are compared to both modeling and previous LSF measurements as verification of the system's capabilities. Many of these measurements are made with reduced photon count rates such that pulse pile-up can be avoided. This approach is common to single photon counting (SPC) measurements. For application to time-series measurements in turbulent flames, the signal level must be increased above SPC guidelines such that the background in the computed PSD does not corrupt the desired information. A pulse pile-up correction will be presented which utilizes a saturated-and-compare technique. This analysis is similar to convolute-and-compare techniques which are commonly used to account for instrumentation response in lifetime measurements. The corrected signal is found to agree with the low-signal measurements in the same laminar flames. With this correction scheme, the system is capable of processing up to 40 million photoelectrons per second. Measurements in a buoyant, flickering, laminar diffusion flame will be presented using the new system, including pulse pile-up correction. This flame has a dominant 15 Hz frequency which is shown to appear in both the lifetime and concentration PSDs. However, the second-harmonic frequency is apparent only in the concentration PSD owing to the shapes of the lifetime and concentration radial profiles. Finally, measurements for turbulent nonpremixed flames will also be presented at a range of Reynolds numbers from 2800 to 19,000. In addition to the PSD, the probability density function (PDF) is computed for each of the reported time series. Both statistics are shown to require quenching corrections for accurate measurements of minor species concentrations.

LASER DIAGNOSTICS OF NITRIC OXIDE INSIDE A 2-STROKE DIRECT INJECTION DIESEL ENGINE

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Nitric Oxide (NO) is one of the main polluting components in the exhaust gases of diesel engines. As such, knowledge of the exact timing and location of the sites where it is produced during the combustion process is of interest for finding means to reduce diesel engine emissions. Laser diagnostics are arguably the most powerful tool for in situ, non-intrusive assessment of local NO densities, as evidenced by several recent publications.

Here we present an evaluation of laser induced fluorescence detection of NO inside a small, optically accessible 2-stroke diesel engine, making an ArF excimer laser (193.4 nm) for excitation and an Optical Multichannel Analyzer (OMA) for spectrally resolved fluorescence detection. The combustion chamber of the engine has been made optically accessible by a 25 mm diameter quartz window mounted centrally in the cylinder head (top window). Two rectangular windows were placed facing each other in the side walls. For the present experiments both the excitation laser and the induced fluorescence passed through the top window. This has the advantage that the excitation laser beam enters the observable volume of the combustion chamber directly, without attenuation.

Dispersed fluorescence spectra are obtained by excitation of the $R_1(26.5)$ transition in the $D^2\Sigma^+(v'=0)\leftarrow X^2\Pi(v''=1)$ band. NO fluorescence bands are observed from the directly excited state, that is the $D^2\Sigma^+(v'=0)\rightarrow X^2\Pi(v''=3,4,5)$. All other bands observed can be attributed to oxygen. At high temperatures (crank angles close to TDC) the absorption spectrum of $O_2$ in the 193 nm wavelength range becomes so dense that it becomes impossible to exclusively excite NO. The fluorescence bands of the two molecules can, however, still be separated. We will present a model to convert this fluorescence yield curve to a NO number density curve, taking into account temperature effects (Boltzmann) and fluorescence quenching as well as laser intensity and fluorescence attenuation. Measurements were performed for different fuels and engine loads; results will be discussed and related to the engine heat release rate and in-cylinder temperature.

A conclusion pertinent to all engine operating conditions studied is that, in this particular engine, the bulk of the NO formation occurs relatively late in the stroke (ca. 25-50° aTDC) and the NO content gradually declines in the colder part of the stroke.

REDUCED EMISSIONS FROM A COMPRESSION IGNITION ENGINE THROUGH BLENDING OF OXYGENATES WITH DIESEL FUEL

A.S. Cheng, J.R. Torres and R.W. Dibble, University of California, Berkeley CA (Work-in-Progress Poster Presented at the *27th International Symposium on Combustion*, Held in Boulder CO, August 1998).

The benefits of oxygenated fuels and synthetic Fischer-Tropsch diesel are being investigated with a Cummins B5.9 diesel engine. The experimental engine is a 5.9 liter, direct-injected, in-line 6-cylinder, turbocharged and aftercooled diesel rated for 175 hp at 2500 rpm. The engine also is equipped for exhaust gas recirculation (EGR). Emissions of particulate matter (PM), oxides of nitrogen ($NO_x$), total hydrocarbons (THC), carbon monoxide (CO) and carbon dioxide ($CO_2$), along with specific fuel consumption (sfc) are being measured during steady state operation at nine engine speed-load conditions and with the different fuels and fuel blends.

Three oxygenated fuels are being evaluated: diethyl ether (DEE), ($C_4H_{10}O$), dimethoxy methane (DMM)($C_3H_8O_2$) and dimethyl ether (DME)($C_2H_6O$). Each of these fuels are being tested in concentrations (by volume in conventional diesel) of 5, 10, 20 and 30 percent. DEE and DMM are also being tested in neat (pure) form, although small amounts of lubricity agents are being

added to prevent wear to fuel system components. Fischer-Tropsch diesel, obtained through synthetic conversion from natural gas feedstock, is being tested in neat form only. Results are being compared to baseline data obtained with conventional diesel fuel.

In addition to measuring PM emissions with standard filter paper techniques, laser light extinction is being investigated as a alternative, fast-response method to measure exhaust gas particle concentration. A He-Ne laser beam (0.6 μm) is passed through the center of a 6 ft section of exhaust pipe, and the resulting laser light intensity is compared to the reference signal to determine particle concentration. Because initial tests show that levels of extinction may be too low (that is, low signal strength, even with a 6 ft path length), laser light scattering will also be investigated. Scattering measurements offer the benefit of providing information on particle size distribution.

Initial experiments show significant reductions in PM emissions for the oxygenated fuel blends. For example, at an engine speed-load condition of 1600 rpm and 320 ft-lbs torque (97 hp), a 30% DMM blend reduced PM emissions by 50% compared to baseline diesel. Significant reductions in THC and CO were also observed. $NO_x$ emission levels were unchanged, but with the reductions in PM emissions, $NO_x$ control strategies could be implemented without producing unacceptable levels of PM. Due to their lower energy density, however, the oxygenated fuel blends result in higher levels of specific fuel consumption.

Additional fuel blend experiments will be conducted using oxygenates labeled with a radioactive carbon-14 tracer. Particle samples collected from these tests will be analyzed to determine the relative contributions to PM from each component of the fuel blend.

### FORMATION MECHANISM OF PAH AND FULLERENES IN PREMIXED BENZENE FLAMES

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The investigation of the chemical mechanism of PAH and particle growth in flames is motivated by data revealing the health effects of combustion generated compounds. A kinetic model describing the formation of PAH up to a mass of 300 amu and of $C_{60}$ and $C_{70}$ fullerenes was developed and tested against experimental data. Data for key radical species such as H and OH and species up to 202 amu, measured in the past by Bittner and Howard using MBMS, were used to test the ability of the present model to predict flame propagation chemistry and the first growth steps. The predictions for larger PAH and fullerenes were tested against concentration profiles measured recently by Grieco et al. in a sooting benzene/oxygen flame by means of state of the art chromatographic techniques. The PAH and fullerene growth process is mainly based on H-abstraction/acetylene-addition, but the addition of larger units such as benzene or phenyl and naphthalene or naphthyl is also considered. Species containing five-membered rings such as acephenanthrylene (202 amu) and cyclopenta[cd]pyrene (226 amu) are included in the mechanism, and the isomerization of acephenanthrylene is shown to be an important pathway for fluoranthene formation. Rate coefficients were evaluated carefully and experimental high temperature data were used whenever possible. Good agreement between prediction and experiment is achieved for PAH formation, but the model fails to predict PAH depletion in the postflame zone. This indicates the presence of additional PAH sinks, such as soot formation, that are not considered in the present model.

## DETERMINATION OF THE CONVERSION DEGREE OF FUEL BOUNDED NITROGEN COMPOUNDS AT THE COMBUSTION OF LIQUID FUELS

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The NO-concentration in the flue gas of furnaces for liquid fuels is the sum of the thermal, prompt and fuel NO formation. Most measures to reduce NO emissions aim mainly on the decrease of the maximum temperature and therefore on the thermal NO formation. Recently the fuel NO formation has become more relevant due to the fact that for modern Low$NO_x$ combustion concepts 30 to 60% of the NO emission result from the conversion of fuelbound nitrogen to NO. The reduction of the concentration of the fuelbound nitrogen in fuels causes a high energy demand during the refining process and has not been realized yet because of economic items.

As a result our investigation provides fundamentals of the conversion degree of fuelbound nitrogen in technical flames. This is useful in the design of new burnerheads which can further reduce NO emission. Additionally, the suitability of model fuels for a standardized test of the emissions in acceptance tests and for the mathematical modeling of the fuel NO-formation is discussed.

In the literature, there are only a few results for the degree of conversion of fuelbound nitrogen compounds. Also, there are no satisfactory analyzing techniques for the determination of specific nitrogen compounds in liquid fuels. Therefore relevant material data for nitrogenated hydrocarbons which are in the boiling range of liquid fuels have been summarized. Additionally nitrogen compounds in liquid fuels were determined with a new analyzing method developed by Severin and David.

Results will be presented which show the influence of the air ratio, the mass fraction of nitrogen, the used basic fuel and chosen nitrogen compound on the conversion degree in technical diffusion and premixed flames.

## EMISSIONS OF $N_2O$ IN FLUIDIZED BED COMBUSTION OF COAL

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Fluidized bed combustion (FBC) has emerged as an environmentally attractive method for burning coal because of low $NO_x$ emissions and optimum conditions for $SO_x$ removal with limestone or dolomite. This is mainly due to the low combustion temperature employed usually between 750 and 950°C. These lower combustion temperatures, however, enhance formation of $N_2O$ ranging from 15 to 300 ppm in comparison with levels observed in pulverized coal combustion boilers at 5 ppm. The higher $N_2O$ levels in fluidized bed combustion systems raise some concern, as it is a potent greenhouse gas and stratospheric ozone layer depleting agent. This study presents a new approach for examining the mechanisms of formation and destruction of $N_2O$ in an incipiently fluidized bed. Combustion gases escaping from the surface of the burning char particle were collected and analyzed for $N_2O$, $NO_x$, CO and $CO_2$ by a Fourier Transform Infrared Spectrometer (FTIR). Experiments were conducted using silica sand particles ranging in size from 200 to 1000 μm at bed temperatures of 500 to 800°C. Results for the coals examined (Wyoming and Colorado coals) show low $N_2O$ levels of 4-7 ppm with $NO_x$ levels of 110-130 ppm. Comparison of experimental results with a single particle char combustion model revealed the dominance of $N_2O$ destruction reactions for large char particles.

LASER INDUCED $C_2$ FLUORESCENCE FROM LASER VAPORIZED SOOT IN LOW PRESSURE LAMINAR PREMIXED ETHYNE/OXYGEN/ARGON FLAMES

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For the validation of detailed chemical models for soot formation and their application to turbulent flames it is necessary to develop a 2-D measuring technique to derive locally resolved soot volume fractions, particle number densities and mean particle radii. In contrast to laminar premixed flames, the extinction technique is not applicable in turbulent systems because of its line-of-sight character. Two methods seem to be suitable to replace the extinction techniques:

- the laser induced incandescence (LII) and
- the laser induced fluorescence of $C_2$ from laser vaporized soot (LIF($C_2$)LVS).

Whereas the first method has been investigated in detail the latter is scarcely mentioned in the literature.

To investigate the LIF($C_2$)LVS technique systematically, the generation of $C_2$ radicals and the excitation of these radicals is separated by means of two consecutive laser pulses. A Nd-YAG laser vaporizes a small part of the soot, which leads to the production of $C_2$ radicals. A delayed dye laser pulse is used to excite the $C_2$ radicals at different transitions of the Swan band system. The experiments were carried out for two laminar premixed ethyne/oxygen/argon flames with different C/O ratios and known soot quantities. The fluorescence signal is spectrally resolved and detected by an intensified CCD camera.

The energies of both pulses have been varied independently and the influence of these changes on the detected signals has been investigated as a function of the height above the burner. For constant vaporization (Nd-YAG with constant output) a linear dependence of the $C_2$ fluorescence with increasing dye-laser energy has been found. On varying the Nd-YAG laser output at constant excitation energy the $C_2$ signal increases with increasing laser energy until a plateau is reached. This laser flux dependence is similar to that measured for the LII signal. A non-sooting flame has also been checked by varying the output energy of the dye laser and determining the energy dependence of the $C_2$ signals. A different fluence dependence has been found. This indicates that the $C_2$ radicals in this case have another source than that one detected in a sooting flame. When calibrating the $C_2$ signals with extinction measurements to obtain absolute soot volume fractions the results are for several measurements in good agreement with the soot volume fractions obtained by LII. Differences are found in some cases for certain laser fluxes and for smaller and larger soot particles (lower and higher heights above the burner). To explain these differences further measurements are in progress.

ANALYSIS OF SOOT SHELL FORMATION IN DROPLET COMBUSTION

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Droplet combustion usually involves the burning of liquid fuels in an oxidizing environment. In the high activation energy limit, the vaporized fuel reacts in a flame-sheet where the reaction heat is liberated. In this laminar diffusion flame structure, soot particles are nucleated at the fuel rich side of the flame. Some experiments in droplet combustion show that the soot may locate in a narrow shell-shaped region between the droplet and the flame. The purpose of this work is to analyze the transport mechanisms which control the dynamics of the soot particles and may lead to the formation of this soot shell accumulation layer.

Due to the presence of strong temperature gradients, thermophoresis drives the particles down the temperature gradient and the particle velocity differs from the local gas velocity. For

a large range of particle sizes, the thermophoretically induced velocity is quite insensitive to particle size and morphology, allowing a soot transport analysis independent of particle size and shape. Assuming that thermophoresis is the only soot particle diffusive transport, the analysis shows that the soot velocity may vanish at a location between the droplet surface and the flame value. However, this shell locus is dynamically unstable. Soot particles generated (or present) in the near droplet region are pushed towards the droplet surface and the soot in the near flame region moves towards the flame and away from the droplet. Then, thermophoresis may lead to the existence of an unstable stagnation locus for the soot particles, but some other phenomena are needed to produce a stable soot shell layer.

For the high temperatures prevailing near the flame, soot radiative heat transfer may be important. The radiation of the individual soot particles generates an overall radial radiative flux. Every particle receives the radiative fluxes produced for the remaining particles except from those shadowed by the presence of the droplet. The incoming radiative flux induces a photophoretic drift of the soot particles. The drift turns out to be in the direction of the droplet. Therefore, a new locus of vanishing soot particle radial velocity may appear near the flame. The photophoretically modified soot velocity and the conditions for the appearance of this stable soot stagnation locus will be reported.

FULLERENE AND SOOT FORMATION IN LOW PRESSURE BENZENE/ACETYLENE/OXYGEN FLAMES

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The formation of fullerenes and soot particles was studied in laminar low pressure flames burning benzene and acetylene as well as mixtures of both with oxygen. Positively charged particles were measured and characterized due to their mass and charge applying a particle mass spectrometer (PMS), which allows detection of particles in the mass range of 600 to 600,000 amu. The influence of the C/O ratio and gas composition on both, the mean particle mass and probability density function of particle mass, was studied. Investigations of a 10% $C_6H_6$/90% $C_2H_2/O_2$ flame have shown that the mass growth of soot particles in mixed flames is similar to the growth behavior in pure $C_2H_2/O_2$ flames. The addition of 10% benzene to acetylene leads to 33 times more charged soot particles compared to the respective amount found in a pure $C_2H_2/O_2$ flame for a specific flow coordinate while the influence on the mean soot mass was found not to be that significant.

Additional studies in which the flow coordinate was chosen to be constant were performed varying the C/O ratio as well as the benzene concentration. Results were compared to the data obtained from measurements on a pure $C_2H_2/O_2$ flame. An increase in the benzene concentration with the C/O ratio fixed at $C/O=0.9$ leads to an increase in the mean soot mass with a coinciding decline in the relative concentration of charged soot particles which are only found up to 50% benzene. For a pure benzene flame, the relative amount of charged fullerenes compared to the amount found in the pure acetylene/oxygen flame increases by a factor of 480. Simultaneous variations of the C/O ratio in the range $0.85 \leq C/O \leq 0.94$ and the benzene concentration influence the soot formation as well as the fullerene formation. In general, more soot particles and fullerenes are formed with an increasing C/O ratio. Variations of the benzene concentration lead to a decreasing soot mass for $C/O < 0.9$ and an increasing soot mass for $C/O \geq 0.9$. As expected, the fullerene mass is not affected by the varying fuel composition. The relative amount of soot particles maximizes when 10% benzene is added to the fuel for all C/O ratios. In contrast, the relative amount of fullerenes shows a constant incline for all variations of the C/O ratio and the benzene concentration.

PARTICLE FORMATION FROM SINGLE DROPLETS OF AQUEOUS SOLUTIONS OF LEAD NITRATE

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The thermal evolution of droplets of aqueous solution of lead nitrate has been studied in a drop-tube furnace which simulates typical conditions for material synthesis through spray pyrolysis and for the thermal destruction of liquid containing waste.

Aqueous droplets (100 μm) of lead nitrate with different salt concentrations have been injected in the drop tube changing the temperature from ambient conditions up to 1200 K, thus covering the processes of droplet evaporation, precursor precipitation within the droplet and thermolysis of the precipitated particles.

Dimensions as well as physico-chemical properties of the droplets/particles have been obtained "in situ" by ultraviolet-visible spectra of scattered light and compared with Scanning Electron Microscopy (SEM) of the sampled material. A plasma generated in the air by a breakdown induced by a Nd:YAG laser has been employed as source for the scattering diagnostics, thus allowing an exceptionally high photon flux in the ultraviolet region where intense and species specific interactions with metal species take place.

Three distinct optical regions characterize aqueous solutions of lead nitrate. A first one, characterized by an extremely strong absorption band around 220 nm, called the "reflective" band, takes into account surface properties of the droplets/particles, a second one with a broad but less intense absorption around 300 nm, called the "refractive" band, gives insights on the inner properties of the droplets and a third, "transparent" band around 400 nm where no significant light interactions occur.

The spray drying process is followed by measuring the light scattered by the droplets in the refractive region. The decrease of the scattering intensity at 300 nm at increasing temperatures is related to the increase of the absorptivity of the aqueous solution due to the selective water evaporation and hence, to the reduction of the droplet size. As the drying process progresses, surface concentration reaches the saturation value and solute is deposited as a solid phase forming a surface crust which grows steadily. At this point in the process of droplet drying, information was retrieved from the signal intensity in the reflective band since it takes into account the light reflected by the particle interface. Two spectral scattering behaviors are detected at temperatures above the salt precipitation within the droplet. On the basis of Mie calculations and SEM measurements these behaviors are attributed to lead nitrate particles with typical diameters of the residual droplets (about 50 μm) and to micrometric sized lead oxide particles.

The effect of salt concentration on the drying process and the thermolysis of lead nitrate to oxide is investigated by changing the salt concentration from very diluted conditions up to almost saturation.

PHASE DOPPLER ANEMOMETRY DETERMINED SODIUM AND POTASSIUM BICARBONATE PARTICLE PROPERTIES IN COUNTERFLOW DIFFUSION FLAMES

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The search for more effective halon replacement agents and alternative fire suppression technologies includes investigations into the suppression properties of aerosols. We recently reported on our investigations of the extinction properties of bicarbonate powders in counterflowing diffusion propane/air flames. This poster extends those studies, examining the

size and velocity distributions of the particles actually delivered to the flames, as well as a determination of the fate of the particles at various strain rates. Powders examined in the current study include potassium bicarbonate ($KHCO_3$) and sodium bicarbonate ($NaHCO_3$) sieved into various size groupings from 38 to 75 μm. A phase Doppler anemometry (PDA) system was used to measure particle velocity, size, and concentration. Particles with sizes that lead to greater residence times near the intersection of the counterflowing fields show a higher suppression effectiveness.

PRODUCTION OF VIBRATIONALLY EXCITED SiO IN THE REACTION OF $SiH_4$ WITH $O(^1D)$

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Compared to the corresponding hydrocarbons, silanes have marked differences in behavior in terms of individual elementary reactions as well as combustion properties. Production of SiO in the title reaction is a typical example of such a contrast. Also, chemistry and molecular physics of SiO vs. CO are of interest.

Experimentally, mixtures of $N_2O$ and $SiH_4$, diluted in He, were irradiated by 193 nm ArF laser pulses in a quasi-static cell, where $N_2O$ was photolyzed to generate the singlet oxygen atom. Progressions of vibrational bands of the SiO ($A^1\Pi$-$X^1\Sigma^+$) transition were monitored by a laser induced fluorescence technique in the wavelength range 230-280 nm. A frequency doubled, YAG pumped conventional OPO (optical parametric oscillator) laser was used for a consecutive sweep over the wide wavelength range, so that the energy distribution of SiO(v) is precisely determined. Temporal profiles of each band exhibit fast rise and relatively slow secondary decay. The former corresponds to the reaction rate of $SiH_4+O(^1D)$ being reported in our previous paper, and the latter is primarily due to vibrational relaxation of SiO. The spectral intensity of the vibrational bands up to v=7 was translated into the vibrational population distribution using known Franck-Condon factors and wavelength dependent sensitivity of the detection system.

The nascent vibrational distribution of SiO was well approximated by a Boltzmann distribution with a vibrational temperature, $T_v$, of 5200(±660) K. That means 5.7% of the total exothermicity of 574 kJ/mol appears in the SiO vibrational mode, when a pair of $H_2$ are assumed as the counterpart of the products. Reported ab initio calculations indicate that the most probable path for the SiO formation is a two-step unimolecular decomposition of internally activated silanol via an HSiOH intermediate. A statistical calculation for the product energy distribution with barrier height corrections yielded $T_v$=5700 K, which is in reasonable agreement with observation. Other pathways, such as one with a $H_2SiO$ intermediate and one that yields H atoms, cannot account for the SiO vibrational excitation due to a higher barrier or lower exothermicity of the products.

Rate constants for the SiO vibrational relaxation at each state ($v \leq 6$) were also evaluated for different collision partners (M). Neighboring transitions ($\Delta v = 1$) were assumed to be dominant in the analysis. When $M = N_2O$, $k_{1\rightarrow 0} = 2.4 \times 10^{-12}$ $cm^3$ $molecule^{-1}s^{-1}$, gradually increasing with v. This is three orders larger than that for He and one order larger than that for $SiH_4$. Probably the high efficiency of $N_2O$ is due to near-resonant V-V energy transfer processes.

IMPACT OF QUARTZ PROBES ON SPECIES PROFILES IN FUEL RICH HYDROCARBON FLAMES

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Molecular beam mass spectrometry based investigations of low pressure premixed flames have proven to yield valuable information about the chemistry of combustion. However, it is well known that the sampling problems of these systems lead to some extent to perturbations of

the studied flame. In an early study Biordi et al. investigated the degree of perturbation of a lean methane flame by several types of sampling probes. By comparing concentration profiles of stable species obtained with different cone types they concluded that a hybrid type sampling cone with tip angle of 40 degrees performs best. Subsequently numerous group used this type of quartz probes.

In preparation of detailed studies of fuel rich hydrocarbon flames we are again interested in the impact of hybrid type quartz cones on the flame structure. Fuel rich flames seem to have a larger tendency of being perturbed by probes and therefore the conclusions of Biordi et al. might not be valid for these flames. Further predictions of species profiles from modeling work are becoming better and better, leading to more stringent requirements for experimental data.

With our MBMS flame chamber apparatus we measure concentration profiles of selected species in three fuel rich flames using three different hybrid type quartz cones: the 'standard' 40 degrees cone, one with a tip angle of 25 degrees and the third one with a tip angle of about 10 degrees. The flames under investigation have the following properties:

1) 18.1% $CH_4$, 28.8% $O_2$, 51.2% Ar ($\Phi$=1.26) at 30 torr with a cold gas velocity of 47.7 cm/s,
2) 16.5% $C_2H_4$, 28.3% $O_2$, 53.3% Ar ($\Phi$=1.75) at 20 torr with a cold gas velocity of 72.5 cm/s,
3) 8.6% *c*-$C_6H_{12}$, 45.8% $O_2$, 44.3% Ar ($\Phi$=1.70) at 40 torr with a cold gas velocity of 54.4 cm/s.

All flames contain in addition a small amount of Neon used as reference gas. The conditions were chosen to create flames with different properties. The ethylene flame shows a significant standoff from the burner surface (about 6 mm) and has an extended luminous zone. In contrast, the cyclohexane flame is very closely attached to the burner surface and its bright reaction zone is very narrow. The properties of the methane flame are in-between the other flames.

Assuming that species profiles obtained with the narrow tip are least affected by perturbation, comparison with profiles measured with the other cones indicates their impacts on the flame structure. We mapped profiles of $O_2$, CO, $CO_2$, $H_2O$ and $C_2H_2$ for this comparison. In the case of radical profiles subsequent reactions in the molecular beam region are more probable to occur in the 10-degree tip due to the lower pumping speed. Differences in signal intensities give an idea of the importance of these secondary reactions during the probing process on experimental results. This will be shown by means of H, OH and $CH_3$ profiles.

## LASER IONIZATION-MASS SPECTROMETRY AS AN ON-LINE SENSOR FOR AROMATICS IN REAL LIFE COMBUSTION PROCESSES: APPLICATION FOR ON-LINE ANALYSIS OF CIGARETTE SMOKE, COMBUSTION FLUE GASES AND PYROLYSIS OFF-GASES

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Resonance-enhanced multiphoton ionization time-of-flight mass spectrometry (REMPI-TOFMS) represents a high selective as well as sensitive analytical technique, well suited for species selective real-time, on-line monitoring of trace gases. A newly designed, mobile REMPI-TOFMS instrument, optimized for field applications has been developed.

The homebuilt, very compact linear time-of-flight mass spectrometer is combined with compact excimer laser (KrF, 248 nm) or a small Nd:YAG laser (fourth harmonic frequency, 266 nm). The data acquisition system allows registration of full mass spectra with a repetition rate of up to 10 Hz. A special effusive molecular beam inlet system was developed for direct inlet of flue gases from, for example, waste incinerators (without memory effects for compounds up to 300 amu). All components are mounted in a movable rack. The achievable on-line detection sensitivity, for example, for naphthalene is about 50 pptv under field measurement conditions (248 nm).

Applications concerning on-line monitoring of combustion byproducts and pyrolysis off-gases are presented. This includes on-line analysis of polycyclic aromatic hydrocarbons (PAH) in the flue gas of a waste incineration plant, headspace analysis of wood gasification products and crude oil (fuel analysis) as well as highly time resolved (single puff resolution) on-line analysis of cigarette smoke (smoking machine and mouthspace analysis).
The application of the on-line REMPI-TOFMS monitor for continuous analysis of dioxin (PCDD/F) indicators in the flue gas of, for example, municipal waste incinerators is explained.

FREQUENCY MODULATION SPECTROSCOPY BEHIND SHOCK WAVES

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For the detection of radicals at high temperatures in the gas phase the difference absorption method is frequently used. In single shot experiments the detection limit of this method is approximately 0.1 to 0.2% absorption. Many kinetic experiments require as low a concentration as possible to reduce the influence of secondary reactions. That is the reason why the detection limit is soon approached. Furthermore no suitable detection method seems to be available for such radicals as $CH_2$ in shock tube measurements. In recent years, several variants of the laser frequency modulated (FM) technique have been developed, which have been successfully used for the detection of weak spectral features. Now, for the first time FM spectroscopy is used for detection of radicals behind shock waves with a higher sensitivity. As a first result, the detection limit of $NH_2$ radicals ($^PQ_{1,N}(7)$ line of the $A^2A_1$-$X^2B_1$ (090-000) transition at 597.375 nm) can be improved by one-and-a-half orders of magnitude. Similar improvements are expected for singlet $CH_2$ detection.
In order to demonstrate the capabilities of this new detection system in combination with a shock tube apparatus several experiments have been performed. We report measurements of

- the unimolecular decomposition of $NH_2$ in an extended temperature range
- the reaction of $NH_2 + H_2$
- the reaction of $NH_2 + NO$, overall rate constant and branching ratios which are important in the $DeNO_x$ process.

Shock tube experiments involving the singlet $CH_2$ radical, which is of special interest in hydrocarbon combustion, are in progress.

SENSITIVE DETECTION OF $NH_2$ IN SHOCK TUBE KINETICS EXPERIMENTS USING FREQUENCY MODULATION SPECTROSCOPY

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The development of more sensitive diagnostics for shock tube kinetics experiments enables measurements at lower initial concentrations and hence, with an increased sensitivity to individual elementary reactions. Although the introduction of laser-based techniques has allowed considerable progress in this direction, classical laser absorption measurements are still subject to the noise caused by the passage of the laser beam through the shock tube, such as scattering and beam steering. Frequency modulation (FM) detection, as a different absorption scheme, is insensitive to these effects and thus allows a considerable improvement in detection sensitivity; so far a factor of 20 has been achieved in our laboratory. We will present experimental details such as reproducible calibration for absolute concentration measurements and the influence of collisional broadening on the frequency modulation signal.
We have applied the FM detection technique to study the branching ratio of the reactions:

$NH_2 + NO \rightarrow H_2O + N_2$ (1a)

$NH_2 + NO \rightarrow HN_2 + OH$ (1b)

These two reactions are the two most influential reactions in determining the efficiency of the non-catalytic removal of NO from exhaust gases by addition of $NH_3$. While there is good agreement in the literature data for the overall rate coefficient of reaction 1, measurements of the branching ratio $\alpha = k_{1b}/k_{1a} + k_{1b}$ show considerable scatter at temperatures above 1000 K. We demonstrate that application of the sensitive frequency modulation technique allows a precise measurement of the branching ratio $\alpha$, with virtually no interference from secondary reactions and independent of the overall rate of reaction 1. The branching ratio is found to increase from 0.4 at 1350 K to 0.6 at 1750 K. This result is in good agreement with a recent modeling study by Glarborg et al.

## PLIF MEASUREMENTS IN A MODEL OIL-FIRED FURNACE WITH HIGHLY PREHEATED, OXYGEN-DEPLETED AIR

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Combustion with highly preheated (T>800 K), oxygen-depleted air has been investigated in both fundamental studies and in practical industrial combustion systems. In industrial systems, regenerative burners are used to produce the inlet air conditions. In these systems, reduced $NO_x$ formation and improvements in the overall furnace combustion efficiency have been noted. More fundamental studies used propane (derived from LPG) and methane gas have recently examined the role of reduced oxygen on the overall flame structure and detailed temperature profiles. In these studies, it was observed that the overall flame luminosity became predominantly green with increasing temperature and decreasing oxygen due to the formation of electronically-excited $C_2$ radicals emitting in the Swan band system near 516 nm. Measurements of both CH and $C_2$ emission showed that the ratio of $C_2$/CH emission increased with air preheat temperature.

This poster will present results from recent studies on oil spray combustion in a model regenerative furnace. Such practical fuels have not been extensively studied in detail previously and are of practical interest. Further, the comparison between the simple gaseous fuels studied earlier and the more complex liquid fuels here is expected to help clarify the role of spray processes, heavier hydrocarbon chemistry, and soot formation in regenerative combustion conditions. Measurements of the $C_2$/CH emission ratio as a function of inlet air conditions show differences compared to the gaseous fuels studies.

Because the emission arises from electronically excited states of the combustion radicals whose chemical production and consumption pathways are poorly understood, we have employed Planar Laser Induced Fluorescence (PLIF) to measure the ground states of the radicals. Instantaneous and time-averaged two-dimensional distributions of these species are expected to more readily clarify their role in the overall flame structure and $NO_x$ emission as a function of regenerative air conditions. In addition to CH and $C_2$ measurements, images of the NO and OH distribution will be reported, adding to the understanding of the overall flame structure and the spatial distribution of NO in the furnace. Temperature profiles and exhaust gas analyses will also be presented. Finally, practical issues associated with industrial, oil-fired combustion with preheated, oxygen-depleted air will be described.

## SPECTROSCOPIC AND TIME RESOLVED INVESTIGATION OF PICOSECOND LASER INDUCED FLUORESCENCE FROM PAH AT ELEVATED TEMPERATURES

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Polyaromatic hydrocarbons (PAH) have been a subject of study for many years and several groups have analyzed the presence of PAH in flames. In situ measurements are generally performed by monitoring the laser induced fluorescence, often spectrally resolved. Studies regarding the spectral behavior of a number of PAH (for example, pyrene and fluoranthene) with respect to temperature in conditions relevant for combustion, have been performed by other groups. For example it has been found that the dual spectral fluorescence from pyrene can be used as a thermometer in combustion environment. However, the spectral profiles of aromatic substances in gas phase are in general almost structureless and broadband and may change with temperature, making it difficult to spectrally select the different species. Measurements of the temporal evolution of the fluorescence emission would in principle increase the possibility to discriminate between different PAH. Decay measurements have been performed by other groups, however, they were conducted at relatively low temperatures compared to real flame conditions.

We have during the last year done picosecond laser induced, spectrally and temporally resolved fluorescence-emission measurements on PAH at atmospheric pressure conditions at temperatures between 150 and 900°C in order to study their temperature and oxygen-quenching behavior. The 266 nm wavelength radiation from a picosecond Nd:YAG was focused with a 1000 mm lens into a flow cell made of quartz. The cell was placed inside an oven and both had optical access for the incoming and outgoing laser beams as well as for the fluorescence emission to be measured at 90°. By an optical arrangement consisting of UV-achromatic lenses, mirrors and filters, the fluorescence emission was focused onto a dual detection system, which included a spectrograph/OMA for the spectral analysis and a photomultiplier tube and a streak camera for the temporal analysis. Fluorescence quenching by oxygen was controlled by mixing the buffer gas (argon or nitrogen) with known amounts of air.

Results on fluorene and naphthalene show that the lifetimes decrease continuously with increasing temperature and that the spectral profiles change, broadening and/or red shifts are observed. Preliminary results indicate that argon and nitrogen may not act in exactly the same way on the decay of the fluorescence emission. Argon was in some cases used instead of nitrogen, for example, for fluorene, which showed relatively low stability to temperature. It was possible to discriminate fluorene from naphthalene in mixtures of the two by observing the decay of the fluorescence emission.

These results and results from measurements on other PAH are presented, both regarding high temperature cell and flame seeding experiments.

## PLANAR LASER INDUCED FLUORESCENCE MEASUREMENTS IN HIGH PRESSURE SPRAY FLAMES

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The extension of planar laser induced fluorescence (PLIF) imaging techniques to elevated pressures is necessary for research and development of advanced gas turbine combustors. We are currently developing a PLIF system for use in high-pressure spray flame environments that simulate gas turbine combustion conditions. In a previous study of high-pressure spray flames, we observed that PLIF images of OH were significantly corrupted by broadband laser induced interference from hydrocarbon intermediates. The concentration of these

hydrocarbon intermediates increased rapidly with pressure, resulting in substantially more interference than occurred at atmospheric pressure. In that work, the burner had poor fuel/air mixing and no preheated air, which tended to increase the levels of hydrocarbon intermediates and soot. Recently, we have constructed an optically-accessible model gas turbine combustor that is operated at 20 atm pressure with inlet air at 500 K and a production liquid fuel injector. This configuration more accurately simulates the conditions of an actual combustor, and it reduces the concentrations of species that corrupt the PLIF signal. In addition, we have implemented a detection scheme that allows the interference to be recorded separately and subtracted from the PLIF signal on a shot-by-shot basis. The detection system includes a multiple-wavelength viewer, which permits simultaneous recording of the interference and PLIF images on different regions of a 1024x256 pixel CCD camera. The LIF is excited by the frequency-doubled output of a Nd:YAG-pumped dye laser. Examples of instantaneous PLIF measurements in our model gas turbine combustor will be presented. These results demonstrate a novel capability for using PLIF imaging diagnostics to study combustion phenomena in a practical combustor.

STRUCTURE OF A HYDROGEN/OXYGEN FLAME DOPED WITH TRIMETHYL PHOSPHATE

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Interest in studying the destruction chemistry of organophosphorus compounds (OPC) in flames is simulated by two reasons. First is the problem of chemical warfare agent disposal by incineration, which has appeared in recent years. The second is associated with some OPC ability to affect the combustion process. The goal of the present research is to provide a more profound understanding of trimethyl phosphate (TMP) destruction chemistry in flames and TMP effects on the $H_2$ oxidation mechanism and to permit subsequent flame structure modeling. As a result, it is necessary to obtain quantitative concentration data on all the flame species (including atoms and free radicals) as a function of the distance from the burner surface. Molecular beam mass spectrometry with electron-impact ionization at 12.9-21 eV and an electron energy spread of ±0.25 eV was used to study the structure of a premixed $H_2/O_2/Ar$ (0.26/0.13/0.61) flame without additives and with 0.2% additive of trimethyl phosphate (TMP), stabilized on a flat flame burner at 47 torr. To calibrate the phosphorus-containing species in the postflame zone, $HOPO_2$, HOPO, $PO_2$ and PO mass peak intensities were measured in stoichiometric and lean flames at different TMP concentrations in the flame. Calibration coefficients for $HOPO_2$, HOPO, $PO_2$ and PO were calculated by solving element balance equations for phosphorus in the postflame zones of different flames. For the first time, orthophosphoric acid was found to be an intermediate product of TMP destruction in flame. Stable components ($H_2$, $O_2$, $H_2O$), atoms and radicals (H,O,OH) were measured as well as organophosphorus compounds - TMP and its destruction intermediates: dimethyl phosphate, dimethyl phosphite, methyl phosphate and methyl phosphite. The calibration coefficients of H, O and OH were estimated by the method based on assumption of partial equilibrium existing in the system of the most "rapid" reactions. Using the results of the intensity profiles measured for all the flame species and the calibration coefficients, the mole fraction profiles of all species, including those of atoms and free radicals were found. The calibration coefficients for some species were determined experimentally, and were estimated for the others. The mechanism of TMP destruction in a $H_2/O_2/Ar$ flame, suggested before, is refined.

SHOCK TUBE STUDY OF THE HIGH TEMPERATURE PYROLYSIS OF ACETALDEHYDE AND OXIRANE
A. Dib, J. DeFelice and J.H. Kiefer, Chemical Engineering Department, University of Illinois at Chicago, Chicago IL (Work-in-Progress Poster Presented at the *27th International Symposium on Combustion*, Held in Boulder CO, August 1998).

Acetaldehyde pyrolysis has been studied behind incident shock waves using the laser-Schlieren (LS) technique over the temperature range 1563 to 2020 K. Three groups of experiments were performed in 2% and 4% acetaldehyde-krypton gas mixtures in the three post-shock pressure ranges of 152-173 torr, 174-219 torr, and 510-552 torr. Pressure dependent rate constants for the initial carbon-carbon bond fission have been derived by modeling the LS data from 46 experiments with an elementary reaction mechanism containing 36 reactions. The fall-off behavior of this bond fission reaction has been successfully modeled with a hindered-rotor Gorin RRKM calculation using a temperature independent $<\Delta E>_{down}$ value of 500 $cm^{-1}$. This RRKM analysis places the unimolecular dissociation of acetaldehyde in the fall-off region close to the low pressure limit.

Branching ratios for hydrogen atom and methyl radical abstraction reactions involving acetaldehyde have been investigated at these high temperatures, and it has been concluded that values of the branching ratios which favor formation of vinoxy radical ($CH_2CHO$) over acetyl radical ($CH_3CO$)

$$\begin{aligned} CH_3 + CH_3CHO &\rightarrow CH_2CHO + CH_4 \\ &\rightarrow CH_3CO + CH_4 \\ H + CH_3CHO &\rightarrow CH_2CHO + H_2 \\ &\rightarrow CH_3CO + H_2 \end{aligned}$$

are consistent with the LS density gradient data. The fate of $CH_2CHO$ in the system has been newly investigated using the transition state frequencies and geometries calculated by Osborn et al. With these, a two-channel master equation calculation has been performed and rate constants for the dissociation of $CH_2CHO$ into ketene, as well as isomerization into $CH_3CO$, have been calculated.

Four additional reactions were added to the acetaldehyde mechanism to successfully model the high temperature pyrolysis of oxirane in krypton. Rate constants for the isomerization of oxirane into acetaldehyde and chemically activated dissociation into methyl and formyl radicals have been derived from the modeling of the LS data and fit with a two channel RRKM calculation. The two channel RRKM calculation predicts the observed favoring of radical formation at low pressures, and the favoring of isomerization to acetaldehyde at high pressures.

A major result from this work is the derivation of incubation times in oxirane pyrolysis. Experiments have been performed which show the sequential processes of vibrational relaxation and dissociation in oxirane.

GAS PHASE RADICAL-RADICAL KINETICS OF THE RADICALS $CH_2F$, $CHF_2$, $CH_3$ AND $C_2H_5$
T. Beiderhase and K. Hoyermann, Institut fur Physikalische Chemie, Universitat Goettingen, and W. Hack, Max-Planck-Institut fur Stromungsforschung, Goettingen, Germany (Work-in-Progress Poster Presented at the *27th International Symposium on Combustion*, Held in Boulder CO, August 1998).

For the description and the prediction of the chemistry of halogenated organic compounds under incomplete combustion like pyrolysis or under poor operating conditions (leading to the formation of undesirable compounds, PICS) the data on elementary reactions of fluorinated radicals are essential. Whereas the self-reactions of $CH_3$ and $CF_3$ radicals lead to the combination products $C_2H_6$ and $C_2F_6$, respectively, the $CH_2F$ and $CHF_2$ radicals can, moreover, show elimination and disproportionation besides. Therefore, the reactions of $CH_2F$ and $CHF_2$ radicals are of theoretical and practical interest.

We want to report on five radical-radical reactions of $CH_2F$, $CHF_2$, $CH_3$ and $C_2H_5$ radicals with relevance to pyrolysis where the priority is set on the measurements of the rate coefficients complemented with primary product detection for a comparison with existing data from final product analysis.

The method used is the discharge-fast-flow-technique, molecular beam sampling, and mass spectrometry applying laser induced multiphoton ionization (especially for radicals) and electron impact ionization.

The mechanism and rate of the reactions of hydrocarbon and fluorinated hydrocarbon radicals in the gas phase have been studied at low pressure ($0.5 \leq p/mbar \leq 2$) and low temperature ($243 \leq T/K \leq 373$). The combination reactions of $CH_2F$ and $CHF_2$ at low pressure lead to HF elimination and stabilization, respectively, in the major reaction routes

$$CH_2F + CH_2F \rightarrow C_2H_3F + HF \qquad (1b)$$

$$k_1 = 7.0(\pm 0.8)x10^{12}(T/298)^{(-3.9\pm1.0)} cm^3/mol{\cdot}s, \ (253 \leq T/K \leq 333)$$

$$CHF_2 + CHF_2 \rightarrow C_2H_2F_4 \qquad (2a)$$

$$k_2 = 2.6(\pm 0.6)x10^{12}(T/298)^{(-1.9\pm0.3)} cm^3/mol{\cdot}s \ (253 \leq T/K \leq 333)$$

The cross combination of $CH_2F$ and $CHF_2$ radicals proceeds via HF elimination from the chemically activated $CH_2FCHF_2$ product

$$CH_2F + CHF_2 \rightarrow C_2H_2F_2 + HF \qquad (3b,c,d)$$

$$k_3(298K) = 4.5(\pm 2.3)x10^{12} cm^3/mol{\cdot}s$$

The mechanisms and rates of the reactions of the $CH_2F$ radicals with the $CH_3$ and $C_2H_5$ radicals were found as

$$CH_2F + CH_3 \rightarrow C_2H_4 + HF \qquad (4b)$$

$$k_4(298K) = 3(\pm 1.5)x10^{13} cm^3/mol{\cdot}s$$

$$CH_2F + C_2H_5 \rightarrow C_3H_6 + HF \qquad (5b)$$

$$k_5(298K) = 1.3(\pm 0.3)x10^{13} \ cm^3/mol{\cdot}s$$

The general mechanism of the hydrocarbon/fluorinated hydrocarbon radical-radical interaction is discussed in the terms governing chemical activation processes (association/redissociation/stabilization/decomposition, elimination).

## OVERALL RATE AND PRODUCT FORMATION STUDIES OF THE REACTION $CH_3+OH$ AT 298, 377 AND 473 K

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The rates of the reactions

$$CH_3 + OH \rightarrow \text{products} \quad (1)$$

and

$$CH_3 + OH \rightarrow {}^1CH_2 + H_2O \quad (1a)$$

are important in hydrocarbon combustion systems in determining the further oxidation pathways of $CH_3$ and thereby the rate of heat release. Both the overall reaction (1) and the $^1CH_2$ forming reaction channel (1a) have attracted significant attention and not less controversy in the literature in the past few years. In a series of recent studies we have applied sensitive and selective direct experimental methods to establish the kinetics of the reactions at 298 K. The present investigations extend the temperature range above room temperature.

Two complementary techniques were used in the experiments. In the low pressure regime it was the fast flow method coupled with laser magnetic resonance detection (DF/LMR) while at higher pressures the laser flash photolysis technique with UV-transient absorption detection (LFP/TAS) was applied. The OH and $CH_3$ radicals were monitored simultaneously both in the

fast flow and the laser flash photolysis experiments. Reaction channel (1a) was determined with the FD/LMR technique by measuring the $^1CH_2$ radical in its triplet form, $^3CH_2$, that was formed via the fast intersystem crossing process in the system. The rate coefficients $k_1$ and $k_{1a}$ were obtained from computer simulations.

The most important findings are the following:

(i) Reaction (1) is characterized by a weak pressure and temperature dependence;

(ii) $^1CH_2$ is the most important reaction product at a few mbar of pressure in the temperature range of 298-473 K;

(iii) The high $^1CH_2$ yields measured indicate that this reaction channel will be important under flame relevant conditions as well, leading to chain propagation in contrast to the chain terminating combination to $CH_3OH$.

## A THEORETICAL STUDY OF THE $C_2H_2$ REACTION WITH $C_2H$ AND $C_3H_3$ RADICALS

L.V. Moskaleva, L.K. Madden and M.C. Lin, Department of Chemistry, Emory University, Atlanta, GA 30322 (Work-in-Progress Poster Presented at the *27th International Symposium on Combustion*, Held in Boulder CO, August 1998).

The reactions of acetylene with unsaturated hydrocarbon radicals such as ethynyl, $C_2H$, and propargyl, $C_3H_3$, are pertinent to the formation of soot in its incipient stages. In the present study we focus on the fragmentation and formation of *n*-$C_4H_3$ and *c*-$C_5H_5$ radicals from the reactions of $C_2H_2$ with $C_2H$ and $C_3H_3$ radicals using different levels of ab initio molecular orbital theory to map the potential energy profiles of the reactions.

The $C_2H + C_2H_2$ reaction initially produces a vibrationally excited *n*-$C_4H_3$ radical which can undergo further fragmentation to give rise to diacetylene, $C_4H_2$, and a hydrogen atom:

$$C_2H + C_2H_2 \underset{-a}{\overset{a}{\leftrightarrow}} n\text{-}C_4H_3^{\dagger} \overset{b}{\rightarrow} C_4H_2 + H$$

Both RCCSD(T)//B3LYP/6-31g(d,p) and G2M(rcc,MP2) calculations yielded a small 2(±1)kcal/mole activation energy for the addition step (a) and a large reverse H-atom addition barrier, $E_{-b}$=11(±2) kcal/mole. The *n*-$C_4H_3$ radical was found to be stable, with respect to $C_4H_2 + H$, by 29(±2) kcal/mole based on the above two methods and a multireference perturbation theory CASPT2(7,7)/6-31g(d,p).

The $C_3H_3 + C_2H_2$ reaction, which involves a sequence of transformations from open-chain to cyclic $C_5H_5$ isomers, was found to take place with 11.6 kcal/mole addition barrier at the CASPT2(6,5)/6-31G(d,p)//B3LYP/6-31g(d,p) level of theory. The most stable *c*-$C_5H_5$, cyclopentadienyl, was calculated to be 77.6 kcal/mole below the $C_3H_3 + C_2H_2$ reactants. Other $C_5H_5$ isomers, *trans*-$C_5H_5$, *cis*-$C_5H_5$, and *isocyclo*-$C_5H_5$, were found to lie at 20.4, 18.4 and 48.5 kcal/mole below the reactants. The transition states connecting those isomers have been found and characterized at the same level of theory.

These ab initio data will be utilized for the rate constant calculations employing multichannel RRKM theory.

## MEASUREMENT OF THE THIRD BODY EFFICIENCY OF WATER FOR THE $H + O_2 + M \rightarrow HO_2 + H_2O$ REACTION AT 35 atm AND 1200 K

R.W. Bates, R.K. Hanson, C.T. Bowman and D.M. Golden, High Temperature Gasdynamics Laboratory, Department of Mechanical Engineering, Stanford University, Stanford, CA 94305 (Work-in-Progress Poster Presented at the *27th International Symposium on Combustion*, Held in Boulder CO, August 1998).

Measurements of the rate of the $H + O_2 + M \rightarrow HO_2 + M$ reaction for $M = H_2O$ at temperatures greater than 900 K exhibit a wide variation in the third-body efficiency of water. Shock tube and flame studies of previous researchers report third-body efficiencies for $H_2O$ compared to argon from 4 to 44. Given the importance of this reaction in many combustion phenomena,

clarification of the third-body efficiency at high temperatures is needed. In addition, existing measurements have been made only near atmospheric pressure, and extension of the data to higher pressures is desirable.

In the work reported here, we extend the technique of Bromly et al. (1995), which is based on observations by Ashmore and Tyler (1962) that a quasi-steady state for $NO_2$ is established in $H_2/O_2$ mixtures containing small amounts of NO for sufficiently high $[NO]/[O_2]$ ratios. Using a shock tube and $Ar^+$ laser absorption of $NO_2$ at 472.7 nm, the third body efficiency of water relative to argon for $H+O_2+M \rightarrow HO_2+M$ at temperatures greater than 1000 K can be determined. Through sensitivity analysis, experimental conditions were chosen so that $NO_2$ plateau levels generated are sensitive only to the known $H+NO_2 \rightarrow NO+OH$ reaction and to $H+O_2+M \rightarrow HO_2+M$ ($M=Ar,H_2O$). Experiments were conducted behind reflected shock waves in a 5 cm internal diameter, stainless steel shock tube using $H_2/O_2/NO/H_2O/Ar$ mixtures. Measured $NO_2$ absorption profiles were quantitatively converted into $NO_2$ mole fraction profiles using measured absorption coefficients. The third-body efficiency of water, relative to argon, was determined by comparison of kinetic modeling fits of the measured $NO_2$ plateaus, using the rate of $H+O_2+M \rightarrow HO_2+M$ as an adjustable parameter, in experiments with and without water addition. Test conditions are centered about 1200 K and 35 atm. Evaluation of the data suggests that the third-body efficiency of water relative to argon, at this temperature and pressure, is consistent with a value of 17.8, found in GRI-Mech v2.11. This result also is in agreement with the work of Ashman and Haynes (1998) from 750-900 K and atmospheric pressure reported at this Symposium.

## RATE CONSTANTS FOR $HO_2$ ADDITION TO PRIMARY, SECONDARY AND TERTIARY CARBON DOUBLE BOND: ETHYLENE, PROPENE AND ISOBUTENE BASE ON AB INITIO CALCULATIONS

C.-J. Chen and J.W. Bozzelli, Department of Chemical Engineering, Chemistry and Environmental Science, New Jersey Institute of Technology, Newark, NJ 07102 (Work-in-Progress Poster Presented at the *27th International Symposium on Combustion*, Held in Boulder CO, August 1998).

The kinetics of $HO_2$ radical addition to the primary, secondary and tertiary carbon double bond of ethylene, propene and isobutene has been studied using ab initio calculations and calculated values are compared with available experimental data. Thermodynamic properties of reactants, adducts and transition state species are determined by ab initio calculations using MP2/6-31G(d), CBS-4 and CBS-q with MP2/6-31G(d) and B3LYP/6-31G(d) optimized geometries. Density function calculations B3LYP/6-31G(d) and B3LYP/6-311+G(3df,2p) are also studied. Kinetic rate parameters for $HO_2$ radical addition to carbon double bonds of olefins are determined from transition state theory. Experimental data and calculated rate constants for addition reactions show similar trends; $HO_2$ radical addition to tertiary carbon double bond ($HO_2$ addition at CD/C2 carbon atom of isobutene) has a lower activation energy than addition to primary or secondary carbon double bond. Comparison of calculated rate constants at CBS-q//MP2/6-31G(d) level with experimental data show good agreement. Transition state structures show a near-planar-ethylene configuration with $HO_2$ addition perpendicular to the plane with a C-O bond length ranging from 1.9365 A(TS of $HO_2$ addition ethylene) to 1.9743 A(TS of $HO_2$ addition at CD/C2 carbon atom of isobutene) and a $\angle$CCO ranging from 90.1° (TS of $HO_2$ addition at CD/H2 carbon atom of isobutene) to 104.07° (TS of $HO_2$ addition at CD/H2 carbon atom of propene) using MP2/6-31G(d) geometry. Energies of activation for $HO_2$ addition to the primary, secondary and tertiary carbon double bond are 10.1, 8.56 and 6.78 kcal/mole, respectively ($HO_2$ addition to ethylene is 12.79 kcal/mole) at CBS-q//MP2/6-31G(d) level. Pre-exponential A-factors are temperature dependent and range from a low of $5.34 \times 10^9$ $cm^3mole^{-1}s^{-1}$, for reaction at 300 K of

$$HO_2 + i\text{-}C_4H_8 \rightarrow (CH_3)_2CCH_2OOH$$

to $4.96 \times 10^{13}$ $cm^3mole^{-1}s^{-1}$, at 1500 K of

$$HO_2 + C_2H_4 \rightarrow CH_2CH_2OOH.$$

## QUANTUM CATALYSIS: THE MODELING OF CATALYTIC TRANSITION STATES

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We present an introduction to the computational modeling of transition states for catalytic reactions. We consider both homogeneous catalysis and heterogeneous catalysis, including organometallic catalysts, enzymes, zeolites and metal oxides, and metal surfaces. We summarize successes, promising approaches, and problems. We attempt to delineate the key issues and summarize the current status of our understanding of these issues. Topics covered include basis sets, classical trajectories, cluster calculations, combined quantum-mechanical/molecular-mechanical (QM/MM) methods, density functional theory, electrostatics, empirical valence bond theory, free energies of activation, frictional effects and nonequilibrium solvation, kinetic isotope effects, localized orbitals at surfaces, the reliability of correlated electronic structure calculations, the role of *d* orbitals in transition metals, transition state geometries, and tunneling.

## *TECHNICAL MEETINGS*

JANUARY 7-9, 1999

*SPECTROSCOPY OF RADICALS AND IONS: HIGH RESOLUTION SPECTROSCOPY GROUP MEETING OF THE ROYAL SOCIETY OF CHEMISTRY*
Southampton, UK.

Information: S. Riaz, The Royal Society of Chemistry, Burlington House, London, W1V 0BN, UK, e-mail: riazs@rsc.org

JANUARY 10-14, 1999

*EUROPEAN WINTER CONFERENCE ON PLASMA SPECTROCHEMISTRY*
Pau, France.

Information: Congress Rive Droite, 28 rue Baudrimont, 33100 Bordeaux, France, 33(556) 32 82 29, Fax 33(556) 32 79 53.

JANUARY 11-14, 1999

*37th AIAA AEROSPACE SCIENCES MEETING AND EXHIBIT*
Reno NV.

Information: R.L. Cook, Mississippi State University, 320 Etheredge Engineering Building, P.O. Drawer MM, Mississippi State, MS 39762, (601) 325 2105, Fax (601) 325 8465, e-mail: cook@dial.msstate.edu

JANUARY 17-22, 1999

*GORDON RESEARCH CONFERENCE ON THE CHEMISTRY OF HYDROCARBON RESOURCES*
Ventura CA.

Topics Include:
- Hydrocarbon Resources in the 21st Century
- Advances in Compositional and Instrumental Approaches to Hydrocarbon Chemistry
- Computational Approaches to Hydrocarbon Reaction Chemistry
- Frontiers of Catalysis in Hydrocarbon Reactions
- High-Temperature Hydrocarbon Chemistry
- Advances in Carbon Materials: Nano-Structures and Catalysts
- Membrane Reactors
- Advances in Methane Conversion Chemistry

Information: J.H. Shinn, Chevron Research and Technology, e-mail: shis@chevron.com or http://www.grc.uri.edu

JANUARY 21-26, 1999

*ANNUAL MEETING OF THE AMERICAN ASSOCIATION FOR THE ADVANCEMENT OF SCIENCE*
Anaheim CA.

Information: E. Cooper, AAAS, (202) 326-6431, Fax (212) 789-0455, e-mail: ecooper@aaas.org, http://www.aaas.org/meetings/scope

JANUARY 22-24, 1999

*INTERNATIONAL SYMPOSIUM ON CLEAN COAL INITIATIVES*
New Delhi, India.

Information: T.N. Singh, Chairman, Organizing Committee, CCI 99 and Director Central Mining Research Institute, Barwa Road, Dhanbad 826 001, Bihar, India, 91(326) 202326/ 203043, EPBX 91(326) 203070/203090, Fax 91(326) 202429/205028,
e-mail: director@cscmri.ren.nic.in; root@cscmri.ren.nic.in

JANUARY 23-29, 1999

*LASE '99: HIGH POWER LASERS AND APPLICATIONS*
San Jose CA.

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Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

JANUARY 24-27, 1999

*13th INTERNATIONAL FORUM ON PROCESS ANALYTICAL CHEMISTRY*
San Antonio TX.

Information: InfoScience Services, Conference Division, 3000 Dundee Road, Suite 409, Northbrook, IL 60062, (847) 291-9161, Fax (847) 291-0097, e-mail: infoscience@ais.net, http://www.ifpac.com

JANUARY 23-29, 1999

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- OPTOELECTRONICS '99 - Integrated Devices and Applications
- SPIE/IS&T's EI '99 - Electronic Imaging: Science and Technology

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

FEBRUARY 6-12, 1999

*PHOTONICS WEST*
San Jose CA.

Information: The International Society for Optical Engineering, SPIE, Meetings Department, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, http://www.spie.org

FEBRUARY 10-12, 1999

*18th IEEE INTERNATIONAL PERFORMANCE, COMPUTING AND COMMUNICATIONS CONFERENCE (IPCCC '99)*
Scottsdale AZ.

Information: N. Malik, General Chairman, IBM Corporation, 11400 Burnet Road, Austin, TX 78758, (512) 838-5106, Fax (512) 838-8378, http://www.ipccc.org/ipccc99/

FEBRUARY 25-26, 1999

*13th ANNUAL TECHNICAL CONFERENCE ON SOLVING ENVIRONMENTAL AND OTHER TECHNOLOGICAL CHALLENGES IN COMBUSTION FOR THE NEXT CENTURY*
Provo UT.

Conference at the Advanced Combustion Engineering Research Center. Topics will Include:
- Combustion Chemistry
- $NO_x$ /Pollutants
- Fine Particles
- Simulations/Validation

Information: Advanced Combustion Engineering Research Center, Brigham Young University, 45 CTB, Provo, UT 84602, (801) 378-4126; Fax (801) 378-3831.

FEBRUARY 28-MARCH 5, 1999

*GORDON RESEARCH CONFERENCE ON GASEOUS IONS, STRUCTURE, ENERGETICS AND REACTION DYNAMICS*
Ventura CA.

Organizing Chairman: T. Baer
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

FEBRUARY 28-MARCH 5, 1999

*GORDON RESEARCH CONFERENCE ON CHEMICAL REACTIONS AT SURFACES*
Ventura CA.

Organizing Chairman: J. Yates
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

MARCH 1-4, 1999

*SAE INTERNATIONAL CONGRESS AND EXPOSITION*
Detroit MI.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

MARCH 7-12, 1999

*PITTCON '99: 50th PITTSBURGH CONFERENCE ON ANALYTICAL CHEMISTRY AND APPLIED SPECTROSCOPY*
Orlando FL.

Information: L. Briggs, Pittsburgh Conference, 300 Penn Center Boulevard, Suite 332, Pittsburgh, PA 15235, (800) 825-3221, Fax (412) 925-3224.

MARCH 8-11, 1999

*24th INTERNATIONAL TECHNICAL CONFERENCE ON COAL UTILIZATION AND FUEL SYSTEMS*
Clearwater FL.

Information: B. Sakkestad, Coal Utilization and Fuel Systems Conference Committee, 1156 Fifteenth Street, NW, Suite 525, Washington, DC 20005, (202) 296 1133, Fax (202) 223 3504, e-mail: barbarasak@aol.com

♦ MARCH 14-17, 1999

*INTERNATIONAL FIRE SAFETY CONFERENCE*
New Orleans LA.

Information: FRCA, 851 New Holland Ave., P.O. Box 3535, Lancaster, PA 17604, (717) 219-5616.

MARCH 14-18, 1999

*1999 SPRING NATIONAL MEETING AND PETROCHEM EXPO OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS*
Houston TX.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 345 East 47th Street, New York, NY 10017, (212) 2705-7338 or (800) 242-4363, http://www.aiche.org

MARCH 15-17, 1999

*TRIPLE JOINT TECHNICAL MEETING OF THE EASTERN/CENTRAL AND WESTERN STATES SECTIONS OF THE COMBUSTION INSTITUTE*
Washington DC.

Information: M.D. Smooke, Becton Laboratory, Room 205, Department of Mechanical Engineering, Yale University, New Haven, CT 06520, (203) 432-4344, Fax (203) 432-6775, e-mail: mitchell.smooke@yale.edu, or
W.J. Pitz, L-14, Lawrence Livermore Laboratory, P.O. Box 808, Livermore, CA 94551, (510) 422-7730, Fax: (510) 422-2644, e-mail: pitz@llnl.gov, http://www.wssci.org/ or http://odie.seas.ucla.edu/WSS/, or
D. Stocker, NASA Lewis Research Center, MS 500-115, 21000 Brookpark Road, Cleveland, OH 44135, (216) 433-2166, Fax (216) 433-8660, e-mail: dennis.stocker@lerc.nasa.gov

MARCH 15-19, 1999

*5th ASME/JSME THERMAL ENGINEERING CONFERENCE: THERMAL ENGINEERING FOR COMBUSTION SYSTEMS AND FIRE SAFETY*
San Diego CA.

Topics will Include:
- Combustion Engines, Furnaces, Incinerators
- Combustion Synthesis, Materials Processing
- Fire Spread, Suppression
- Measurement, Modeling Methods
- Fundamental Physical Processes in Flames

Information: T. Simon, Department of Mechanical Engineering, University of Minnesota, 111 Church Street, SE, Minneapolis, MN 55455, (612) 625 5831, Fax (612) 624 5230, e-mail: tsimon@me.umn.edu, http://www.asme.org/conf/A-JSME98/index.htm

MARCH 18-19, 1999

*2nd POLLUTION PREVENTION TOPICAL WORKSHOP HOSTED BY THE ENVIRONMENTAL DIVISION OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS*
Houston TX.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 345 East 47th Street, New York, NY 10017, (212) 2705-7338 or (800) 242-4363, http://www.aiche.org, or Contact Conference Chairman S. Butner at butner@battelle.org or J. Cramer at (212) 591-7950, e-mail: josec@aiche.org, or Program Details at http://www.seattle.battelle.org/AICHE98/

MARCH 21-25, 1999

*217th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
Anaheim CA.

Division of Fuel Chemistry:
- Molecular Approaches to CH Activation and Selective Oxidation of Alkanes
  R. Periana, Catalytica Advanced Technologies, 430 Ferguson Drive, Building 3, Mountain View, CA 94043-5272, (650) 940-6396, Fax (650) 968-7129, e-mail: rap@mv.catalytica-

inc.com; R.H. Crabtree, Department of Chemistry, Yale University, 225 Prospect Street, New Haven, CT 06520-8107, (203) 432-3925, Fax (203) 432-6144, e-mail: crabtree@minerva.cis.yale.edu

- Renewable Fuels and Chemicals
  R. Evans, National Renewable Energy Laboratory, 1617 Cole Boulevard, Golden, CO 80401-3393, (303) 384-6284, e-mail: evansb@tcplink.nrel.gov
- Chemistry of Reactive Intermediates and Modeling in Hydrocarbon Conversion
  J.A. Franz; M.T. Klein, Department of Chemical Engineering, University of Delaware, Newark, DE 19716
- New Catalysts for Hydrogenation and Hydrocracking of Fuels
  M.E. Davis, California Institute of Technology, Pasadena, CA 91125, (818) 395-6811, e-mail: mdavis@macpost.caltech.edu; S. Zones, Chevron, (510) 242-3524
- Role of Water in Organic Reactions
  M. Lewan, U.S. Geological Survey, Box 25046 MS 977, Denver Federal Center, Denver, CO 80255, (303) 236-9391, e-mail: mlewan@bpgsvr.cr.usgs.gov; G.D. Cody, Geophysical Laboratory, Institute of Washington, 5251 Broad Branch Road, N.W., Washington, DC 20015, (202) 686-2410 ext. 2479, e-mail: cody@gl.ciw.edu

Division of Petroleum Chemistry:

- Lower Alkane Oxidation
  U.S. Ozkan, Department of Chemical Engineering, Ohio State University, 140 W. 19th Avenue, Columbus, OH 43210, (614) 292-6623, Fax (614) 292-3769, e-mail: ozkan.1@osu.edu

Division of Physical Chemistry:

- Physical Chemistry at High Pressure and Temperature
  A.P. Alivisatos, Department of Chemistry, University of California, Berkeley, CA 94720, (510) 643-7371, Fax (510) 642-6911, e-mail: alivis@uclink4.berkeley.edu
- Atmospheric Chemistry
  C.E. Miller, Department of Chemistry, Haverford College, Haverford, PA 19041, (610) 896-1388, Fax (610) 896-4904, e-mail: cmiller@haverford.edu
- Unimolecular Reactions and Intramolecular Dynamics
  S.J. Klippenstein, Chemistry Department, Case Western Reserve University, Cleveland, OH 44106, e-mail: sjk5@po.cwru.edu

Complete Information at http://www.acs.org/meetings/ anaheim/welcome.htm

MARCH 21-26, 1999

*23rd ENGINEERING FOUNDATION CONFERENCE ON STATIONARY SOURCE SAMPLING AND ANALYSIS FOR AIR POLLUTANTS*
Ventura CA.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441.

MARCH 22-26, 1999

*AMERICAN PHYSICAL SOCIETY CENTENNIAL MEETING*
Atlanta GA.

Information: Meetings Department, American Physical Society, One Physics Ellipse, College Park, MD 20740, (301) 209-3286, Fax (301) 209-0866, e-mail: meetings@aps.org

♦ MARCH 25-26, 1999

*ADVANCED MARINE MACHINERY SYSTEMS WITH LOW POLLUTION AND HIGH EFFICIENCY*
Newcastle upon Tyne, UK.

Information: A. Evripidou, The Institute of Marine Engineers, 76 Mark Lane, London EC3R 7JN, UK, (171) 481-8493, Fax (171) 488 1854, e-mail: ae@imare.org.uk

♦ MARCH 29-APRIL 2, 1999

*FRONTIERS IN SCIENCE AND TECHNOLOGY: SCIENCE OF CLIMATE*
La Jolla CA.

Information: Frontier Scientific Research Conference, La Jolla International School of Science, Institute for Advanced Physical Studies, 7596 Eads Ave., La Jolla, CA 92038, e-mail:wisdom@stefan-university.edu

♦ APRIL 7-9, 1999

*10th ANNUAL UNITED STATES HYDROGEN MEETING OF THE NATIONAL HYDROGEN ASSOCIATION*
Vienna VA.

Information: National Hydrogen Association, 1800 M Street, N.W., Suite 300, Washington DC, 20036, (202) 223-5547.

♦ APRIL 9-10, 1999

*NEW ENGLAND SECTION SPRING MEETING OF THE AMERICAN PHYSICAL SOCIETY*
Yale University, New Haven CT.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ APRIL 11-14, 1999

*13th TOPICAL CONFERENCE ON APPLICATIONS OF RADIOFREQUENCY POWER PLASMAS*
Annapolis MD.

Information: S. Bernabei, Princeton Plasma Physical Laboratory, P.O. Box 451, Princeton, NJ 08543, e-mail: sbernabei@pppl.gov

♦ APRIL 11-14, 1999

*ASME CONFERENCE ON RENEWABLE AND ADVANCED ENERGY SYSTEMS FOR THE 21st CENTURY*
Lahaina, Maui HI.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

♦ APRIL 12-15, 1999

*40th AIAA/ASME/ASCE/AHS/ASC STRUCTURES, STRUCTURAL DYNAMICS AND MATERIALS CONFERENCE*
St. Louis MO.

Information: Meetings Department, American Institute of Aeronautics and Astronautics, 1801 Alexander Bell Drive, Suite 500, Reston, VA 20191, (703) 264-7500 or (800) 639-2422, e-mail: custserv@aiaa.org, http://www.aiaa.org

♦ APRIL 13-16, 1999

*13th INTERNATIONAL CONFERENCE ON OPTICAL FIBER SENSORS*
Kyongju, South Korea.

Information: OFS-13 Secretariat, Department of Physics, KAIST, 373-1 Kusong-dong, Yusong-gu, Taejon 305-701, South Korea, e-mail: ejsohn@cais.kaist.ac.kr

♦ APRIL 14, 1999

*JOINT MEETING OF THE BRITISH SECTION OF THE COMBUSTION INSTITUTE AND UKELG: INDUSTRIAL COMBUSTION HAZARDS*

Information: J. Griffiths, School of Chemistry, University of Leeds, Leeds LS2 9JT, UK, 011-44(1132) 336462, Fax (1132) 336565.

♦ APRIL 14-15, 1999

*THE UK COAL RESEARCH FORUM ANNUAL MEETING*
London UK.

Will Include Workshops on
- Fundamental Coal Research
- Conventional and Advanced Power Generation

Information: D.J.A. McCaffrey, CRE Group Ltd., Stoke Orchard, Cheltenham, Gloucester GL52 4RZ, UK, (1242) 673361, Fax (1242) 677010.

APRIL 14-16, 1999

*4th INTERNATIONAL MEETING ON CATALYTIC COMBUSTION*
San Diego CA.

Information: http://www.catalytica-inc.com/WCC4

♦ APRIL 19-22, 1999

*CHAPMAN CONFERENCE ON ATMOSPHERIC SCIENCE ACROSS THE STRATOSPHERE*
Annapolis MD.

Information: American Geophysical Union, 2000 Florida Avenue N.W., Washington, DC 20009, (202) 462-6900, (800) 966-2481, Fax (202) 328-0566, Service and Information Center: service@agu.org, http://www.agu.org

APRIL 19-23, 1999

*2nd INTERNATIONAL SYMPOSIUM ON HEAT AND MASS TRANSFER UNDER PLASMA CONDITIONS: PLASMA '99*
Antalya, Turkey.

Topics will Include:

- Turbulence Phenomena in Thermal Plasmas
- Plasma Transport Properties of Complex Mixtures Including Diffusion
- Radiative Transport under Plasma Conditions
- Non-equilibrium Effects in Thermal Plasma Systems
- Plasma-Wall Boundary Layers and Electrode Erosion Phenomena
- Electromagnetically Induced Flow Effects in Plasma Systems
- Plasma Particulate Interactions
- Transport Processes in Dusty Plasmas
- Rapid Solidification During Plasma Deposition
- Particle Nucleation and Growth in Plasma Reactors
- Waste Treatments and On-line Controls in Connection with Environmental Regulations
- Material Behavior under Extremely High Heat Fluxes ($>10^9$ $Wm^{-2}$)
- Flash Evaporation
- Diagnostic Techniques in Plasma Chemical Applications, in Dusty Plasmas, in Particle Flattening and Splat Cooling
- On-line Control in Plasma Processes
- New Branches of Plasma Physics and Transport Phenomena (MAD, Improved MHD, EHD, DL and DL Currents)

Information: P. Fauchais, Faculte des Sciences, Universite de Limoges, 123 Avenue A. Thomas, 87060 Limoges Cedex-France, (33-5) 55 45 74 21, Fax (33-5) 55 45 72 11, e-mail: fauchais@unilim.fr, or F. Arinc, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210 5214, Fax (90) 312-210 1331, e-mail: arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr
Deadline: 4-Copies of Extended Abstract to P. Fauchais (above) by October 15, 1998, Abstracts for Poster Presentations by January 30, 1999.

APRIL 23-24, 1999

*NEW YORK SECTION SPRING MEETING OF THE AMERICAN PHYSICAL SOCIETY*
Murray Hill NJ.

Information: R.S. Galik, Vice Chair, 108 Newman Laboratory, Cornell University, Ithaca, NY 14853, (607) 255 3633, Fax (607) 254 4552, e-mail: rsg@ins62.ins.cornell.edu

APRIL 25-30, 1999

*CORROSION '99: 54th NACE INTERNATIONAL CONFERENCE AND EXHIBITION*
San Antonio TX.

Information: Meetings Department, NACE, P.O. Box 218340, Houston, TX 77084, (281) 228-6223, Fax (281) 228-6300, e-mail: msd@mail.nace.org, http://www.nace.org

♦ APRIL 26-30, 1999

*FRONTIERS IN SCIENCE AND TECHNOLOGY: AEROSOL SCIENCE AND TECHNOLOGY*
La Jolla CA.

Information: Frontier Scientific Research Conference, La Jolla International School of Science, Institute for Advanced Physical Studies, 7596 Eads Ave., La Jolla, CA 92038, e-mail:wisdom@stefan-university.edu

♦ APRIL 27-29, 1999

*9th ANNUAL MEETING OF THE HALON OPTIONS TECHNICAL WORKING CONFERENCE*
Albuquerque NM.

Topics will Include:

- Halon Replacements and Alternatives
- Advanced Technologies
- Toxicity Issues
- Halon Bank Management and Destruction
- Fire Suppression Testing
- Regulatory and Environmental Issues
- Inert Gases
- Advanced Agents
- Agent Decomposition
- Laboratory Testing
- Misting Technologies
- Particulate Aerosols
- Basic Research

Special Sessions are Planned on:

- $CF_3I$
- Bromoalkane Blends
- Next-Generation Fire Suppression Technology Program
- Informed Decisions: A User's Perspective

Information: R.E. Tapscott, Director, Center for Global Environmental Technologies, University of New Mexico, 901 University Boulevard SE, Albuquerque, NM 87106, (505) 272-7252, Fax (505) 222-8230, e-mail: tapscott@nmeri.unm.edu

♦ APRIL 30-MAY 1, 1999

*OHIO SECTION SPRING MEETING OF THE AMERICAN PHYSICAL SOCIETY*
Flint, MI.

Information: Bahram Roughani, e-mail: broughan@nova.gmi.edu

♦ MAY 2-5, 1999

*4th ITALIAN CONFERENCE ON CHEMICAL AND PROCESS ENGINEERING*
Florence, Italy.

Information: AUDIC ICheaP-4 Secretariat, Piazza Morandi 2, 20121 Milano, Italy, (02) 760-21175, Fax (02) 799644, e-mail: aidic@aidic.it, Web Site: http://www.aidic.it

♦ MAY 2-7, 1999

*195th MEETING OF THE ELECTROCHEMICAL SOCIETY*
Seattle WA.

Symposia Include among Others:
- General Session on Corrosion
- Fullerenes: Chemistry, Physic s and New Directions

Information: http://www.electrochem.org/meetings

♦ MAY 3-6, 1999

*INTERNATIONAL FUELS AND LUBRICANTS SPRING MEETING AND EXPOSITION OF THE SOCIETY OF AUTOMOTIVE ENGINEERS*
Dearborn MI.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

♦ MAY 4-7, 1999

*5th ASIAN CONFERENCE ON ANALYTICAL SCIENCES*
Xiamen, China.

Information: Sun Dahai, Department of Chemistry, Xiamen University, Xiamen 361005, China, Fax 86(592) 218 6401, e-mail:asianalysis@xmu.edu.cn, Web Site: http://www.xmu.edu.cn/sedc/english/confer.htm

MAY 9-12, 1999

*2nd ASIA-PACIFIC CONFERENCE ON COMBUSTION*
Tainan, Taiwan

Topics will Include:
- Gaseous Combustion
- Liquid Fuels, Droplet and Spray Combustion
- Solid Fuels and Coal Combustion
- Reaction Kinetics of Combustion, Pollutant formation and Control
- Laminar Flame Combustion
- Turbulent Premixed, Partially Premixed and Non-Premixed Combustion
- Detonations and Supersonic Combustion
- Internal Combustion Engines, Gas Turbine Engines and Rocket Engines
- Stationary Combustion Systems and Incineration
- Fire Research

- Material Synthesis and Catalytic Combustion Manufacturing
- Combustion Modeling and Computational Combustion
- Combustion in Microgravity Systems

Information: T.-H. Lin, Department of Mechanical Engineering, National Cheng Kung University, 1 Ta-Shue Road, Tainan, Taiwan 701, 886(6)2757575, ext. 62167, Fax 886(6)2352973, e-mail: thlin@mail.ncku,edu.tw

MAY 10-12, 1999

*21st INTERNATIONAL POWER SOURCES SYMPOSIUM*
Brighton UK.

Information: R.D. Bailey, Crundalls, Gedges Hill, Matfield, Kent TN12 7EA, UK, (44)1892 723408, Fax (44)1892 723874, e-mail: ipss@marketdevelopco.demon.co.uk

♦ MAY 10-14, 1999

*THE 1999 INTERNATIONAL CONFERENCE ON INCINERATION AND THERMAL TREATMENT TECHNOLOGIES*
Orlando FL.

Information: Conference Coordinator, L.B. Cohen, University of California, EH&S, 300 University Tower, Irvine, CA 92697, (949) 824-5859, Fax (949) 824-1900, e-mail: lbarnow@uci.edu

MAY 16-19, 1999

*ASME FLUIDIZED BED COMBUSTION CONFERENCE*
Savannah GA.

Information: Meetings Department, ASME, 345 E. 47th St., New York, NY 10017, (212) 705-7037, Fax (212) 705-7143.

♦ MAY 17-19, 1999

*7th ASME ANNUAL NORTH AMERICAN WASTE-TO-ENERGY CONFERENCE*
Tampa FL.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

MAY 17-19, 1999

*32nd MIDDLE ATLANTIC REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
Madison NJ.

Information: G. Heinz, 30 Bunker Hill Run, East Brunswick, NJ 08816, (732) 257 5754.

♦ MAY 18-20, 1999

*THE 5th INTERNATIONAL MICROGRAVITY COMBUSTION WORKSHOP*
Cleveland OH.

Information: A. Heyward, Outreach Programs Manager, National Center for Microgravity Research on Fluids and Combustion, NASA Lewis Research Center, Cleveland OH, (216) 433-8173, e-mail: Ann.O.Heyward@lerc.nasa.gov, http://www.ncmr.org/events/workshop.html

MAY 18-21, 1999

*JOINT MEETING OF THE BRITISH, GERMAN AND FRENCH SECTIONS OF THE COMBUSTION INSTITUTE*
Nancy, France.

Information: C. Poulain (CPIC), 33(0)383301161, Fax 33(0)383175215, e-mail: cpic@ensic.u-nancy.fr

MAY 21-22, 1999

*1st MEETING OF THE NORTHWEST SECTION OF THE AMERICAN PHYSICAL SOCIETY*
Vancouver BC, Canada.

Information: E. Henley, e-mail: henley@nucthy.phys.washington.edu

MAY 23-28, 1999

*CONFERENCE ON LASERS AND ELECTRO-OPTICS (CLEO 99) AND THE QUANTUM ELECTRONICS AND LASER SCIENCE CONFERENCE (QELS 99)*
Baltimore MD.

Information: Information: Meetings Department, Optical Society of America, 201 Massachusetts Avenue, Washington, DC 20036, (202) 223-8130.

♦ MAY 30-JUNE 2, 1999

*82nd CANADIAN SOCIETY FOR CHEMISTRY CONFERENCE AND EXHIBITION*
Toronto, Canada.

Information: P. Sundar Sundararajan, Xerox Research Center of Canada, 2660 Speakman Drive, Mississauga, Ontario L5K 2L1, Canada, (905) 823-7091 ext. 219, e-mail:Sundar.Sundararajan@crt.xerox.com

♦ JUNE 6-10, 1999

*5th INTERNATIONAL CONFERENCE ON CHEMICAL STRUCTURES*
Noordwijkerhout, The Netherlands.

Information: G. Grethe, c/o MDL Information Systems Inc., 14600 Catalina Street, San Leandro, CA 94577, (510) 895-1313 ext. 1430, Fax (510) 614-3638, e-mail:guenter@mdli.com

♦ JUNE 6-11, 1999

*GORDON RESEARCH CONFERENCE ON OSCILLATIONS AND DYNAMIC INSTABILITIES IN CHEMICAL SYSTEMS*
Il Ciocco, Italy.

Organizing Chairperson: R. Larter
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

♦ JUNE 7-8, 1999

*SPQ-99: SPECTROSCOPY IN PROCESS AND QUALITY CONTROL*
East Brunswick NJ.

Information: R. Vallari, Advanstar Communications, 101 Fieldcrest Avenue, Raritan Plaza III, Edison, NJ 08837, (732) 225-9500, Fax (732) 225-0211, e-mail: rvallari@advanstar.com

♦ JUNE 7-10, 1999

*ASME TURBO EXPO '99: LAND, SEA AND AIR, 44th ASME INTERNATIONAL GAS TURBINE AND AEROENGINE TECHNICAL CONGRESS EXPOSITION AND USERS SYMPOSIUM*
Indianapolis IN.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

♦ JUNE 7-11, 1999

*14th INTERNATIONAL CONFERENCE ON LASER SPECTROSCOPY ICOLS '99*
Innsbruck, Austria.

Topics will Include:
- Atomic and Molecular Laser Spectroscopy
- Precision Spectroscopy
- Laser Cooling and Trapping
- Quantum Optics
- Matter Wave Optics and Interferometry
- Nonlinear Optics and Spectroscopy
- Ultrafast and Strong Field Phenomena
- New Laser Sources
- Applications of Laser Spectroscopy
- Bose-Einstein Condensation and Atom Lasers

Information: D. Leibfried, Institut f. Experimentalphysik, Universitaet Innsbruck, Technikerstrasse 25, A-6020 Innsbruck, Austria, Fax (43) 512-507-2952, e-mail: icols99@uibk,ac.at, http://physics.uibk.ac.at/ICOLS99

♦ JUNE 13-18, 1999

*GORDON RESEARCH CONFERENCE ON ATMOSPHERIC CHEMISTRY*
Salve Regina University, Newport RI.

Organizing Chairpersons: W.H. Brune and J.E. Penner
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

♦ JUNE 13-18, 1999

*47th CONFERENCE ON MASS SPECTROMETRY AND ALLIED TOPICS*
Dallas TX.

Information: J. Sjoberg, American Society for Mass Spectrometry, 1201 Don Diego Avenue, Santa Fe, NM 87505, (505) 989-4517, Fax (505) 989-1073, e-mail: asms@asms.org

JUNE 14-18, 1999

*LASER '99*
Munich, Germany.

Information: Messe Munchen GmbH, Messegelande, D-80325 Munchen, Germany, 49(0) 89 51 070, Fax 49(0) 89 51 07 506, e-mail: info@messe-muenchen.de

♦ JUNE 16-20, 1999

*4th INTERNATIONAL CONFERENCE ON DISSOCIATIVE RECOMBINATION*
Stockholm, Sweden.

Information: M. Larsson, Department of Physics, Stockholm University, Box 6730, S-11385 Stockholm, Sweden, e-mail: mats.larsson@physto.se

JUNE 19-23, 1999

*MEDITERRANEAN COMBUSTION SYMPOSIUM OF THE COMBUSTION INSTITUTE AND THE INTERNATIONAL CENTER FOR HEAT AND MASS TRANSFER*
Antalya, Turkey.

Topics will Include:
- Stationary Sprays and Gas Combustion Systems
- Combustion of Solid Fuels PF, FBC and Waste
- Internal Combustion Engines
- Optical Diagnostics and Radiative Transfer
- Flame Dynamics and Turbulence
- Pollutants
- Fire/Explosions
- Kinetics

Information: F. Arinc, Secretary General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210 1429, Fax (90) 312-210 1331, e-mail: arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr

Deadline: Submit Camera Ready Copy of the Full Paper together with Three Additional Copies, Plus One 3.5" Floppy Disk Containing in a Word File only the Title, Authors, Affiliation and Abstract by November 1, 1998 to Martine van Hapert, Istituto di Richerche sulla Combustione - CNR, P.le Tecchio, 80, 80125 Napoli, Italy, (39) 81-768 2263, Fax (39) 81-593 6936, e-mail: martine@irc.na.cnr.it
Work in Progress Presentations: Send One Camera Ready Abstract and 2-Copies by February 1, 1999 to Filiz Ozler, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210 5213, Fax (90) 312-210 1331, e-mail: ichmt@metu.edu.tr

JUNE 20-22, 1999

*54th NORTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
Portland OR.

Information: T. Dunne, 3203 Southeast Woodstock Boulevard, Portland, OR 97202, (503) 777-7207, Fax (503) 777-7769.

♦ JUNE 20-24, 1999

*35th AIAA/ASME/SAE/ASEE JOINT PROPULSION CONFERENCE AND EXHIBIT*
Los Angeles CA.

Information: Meetings Department, American Institute of Aeronautics and Astronautics, 1801 Alexander Bell Drive, Suite 500, Reston, VA 20191, (703) 264-7500 or (800) 639-2422, e-mail: custserv@aiaa.org, http://www.aiaa.org

♦ JUNE 20-25, 1999

*GORDON RESEARCH CONFERENCE ON LASER DIAGNOSTICS FOR COMBUSTION RESEARCH*
Il Ciocco, Italy.

Organizing Chairpersons: K. Kohse-Hoinghaus and J.B. Jeffries
Information: J.B. Jeffries, SRI International, Molecular Physics Laboratory, 333 Ravenswood Avenue, Menlo Park, CA 94025, (650) 859-6341, Fax (650) 859-6196, e-mail: jeffries@mplvax.sri.com, http://pc1.chemie.uni-bielefeld.de/gordon
Deadline: Posters, February 15, 1999.

JUNE 21-23, 1999

*31st CENTRAL REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
Columbus OH.

Information: J. Parson, Chemistry Department, Ohio State University, 100 W. 18th Avenue, Columbus, OH 43210, (614) 292-3267, Fax (614) 292-1685, e-mail: parson2@osu.edu

♦ JUNE 21-24, 1999

*FOURIER TRANSFORM SPECTROSCOPY: NEW METHODS AND APPLICATIONS*
Santa Barbara CA.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org

♦ JUNE 21-25, 1999

*COURSE ON THE FUNDAMENTALS OF INTERNAL COMBUSTION ENGINES: PERFORMANCE, EFFICIENCY AND EMISSIONS*
MIT, Cambridge MA.

Organized by W.K. Cheng and J.B. Heywood
Information: Professional Institute, Room 8-201, Massachusetts Institute of Technology, Cambridge, MA 02139, (617) 253-2101, Fax (617) 253-8042, e-mail: professional-institute@mit.edu, Web Site: http://web.mit.edu/professional/summer/
Course Fee: $2250.

JUNE 21-26, 1999

*28th NORTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
Potsdam NY.

Information: P. Zuman, Department of Chemistry, Potsdam University, Potsdam, NY 13699, (315) 268-2340.

JUNE 27-30, 1999

*PULSED POWER CONFERENCE*
Monterey CA.

Information: C. Stallings, Physics International, 2700 Merced Street, San Leandro, CA 94577, e-mail: chstallings@corp.olin.com

JUNE 27-30, 1999

*6th INTERNATIONAL CONGRESS ON TOXIC COMBUSTION BYPRODUCTS*
Karlsruhe, Germany.

Information: e-mail: pic22@ict.uni-karlsruhe.de, http://www.ict.uni-karlsruhe.de/pic99/
Deadline: 2-Page Abstract Due by December 31, 1998, Final Paper June 1999 and will be Published in *Combustion Science and Technology*.

♦ JUNE 27-JULY 2, 1999

*GORDON RESEARCH CONFERENCE ON GRAVITATIONAL EFFECTS IN PHYSICO-CHEMICAL SYSTEMS*
New England College, Henniker NH.

Organizing Chairman: R.F. Sekerka
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

♦ JUNE 27-JULY 2, 1999

*GORDON RESEARCH CONFERENCE ON PHOTOACOUSTIC AND PHOTOTHERMAL PHENOMENA*
Colby-Sawyer College, New London NH.

Organizing Chairman: J. Power
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

♦ JUNE 28-JULY 1, 1999

*17th APPLIED AERODYNAMICS CONFERENCE/14th AIAA COMPUTATIONAL FLUID DYNAMICS CONFERENCE/30TH AIAA FLUID DYNAMICS CONFERENCE/30TH AIAA PLASMADYNAMICS AND LASERS CONFERENCE/33RD AIAA THERMOPHYSICS CONFERENCE*
Norfolk VA.

Information: Meetings Department, American Institute of Aeronautics and Astronautics, 1801 Alexander Bell Drive, Suite 500, Reston, VA 20191, (703) 264-7500 or (800) 639-2422, e-mail: custserv@aiaa.org, http://www.aiaa.org

JUNE 29-JULY 1, 1999

*INTERFLAM '99*
Edinburgh, Scotland.

Topics will Include:
- Advances in Detection, Extinction and Suppression - Halon Replacement
- Applied Fire Safety Science and the Fire Service
- Comparison of Computer Models with Experimental Data
- Disaster Mitigation and Large Fire Studies (Forest Fires)
- Education
- Fire Behavior of Materials
- Fire Dynamics - Flame Spread and Heat Release Studies
- Fire Risk Assessment
- Harmonization of Fire Safety Standards
- Heat Transfer from Flames
- Human Behavior and Evacuation Modeling
- Interpretation of Small Scale Test Datea
- Properties of Combustion Products
- Performance Based Codes
- Structural Behavior

Information: C. Franks, Conference Secretariat, Interscience Communications Ltd., West Yard House, Guildford Grove, Greenwich, London Se10 8JT, UK, 44(181)692 5050, Fax 44(181)692 5155, e-mail: intercomm@dial.pipex.com.uk

♦ JULY 4-6, 1999

*2nd INTERNATIONAL SYMPOSIUM ON INCINERATION AND FLUE GAS TREATMENT TECHNOLOGIES*
Sheffield UK.

Information: J. Black, Conference Department, IChemE, 165-189 Railway Terrace, Rugby CV21 3HQ, Warwickshire, UK, 011-44 (1788) 578214, Fax (1788) 577182, e-mail: jblack@icheme.org.uk

♦ JULY 5-7, 1999

*15th ANNUAL CONFERENCE ON LIQUID ATOMIZATION AND SPRAY SYSTEMS*
Toulouse, France.

Information: Secretariat ILASS-Europe '99, ONERA-Centre de Toulouse, 2 Av. Edourd Belin, BP 4025, 31055 Toulouse Cedex, France, (5) 62 25 25 82, Fax (5) 62 25 25 83, e-mail: gerard.lavergne@onecert.fr

JULY 5-9, 1999

*STEREOCHEMISTRY AND CONTROL IN MOLECULAR REACTION DYNAMICS. A DISCUSSION COMPARING FREQUENCY, TEMPORAL AND PHASE CONTROL STRATEGIES TO PROBE ELEMENTARY CHEMICAL PROCESSES: A FARADAY DISCUSSION OF THE ROYAL SOCIETY OF CHEMISTRY*
Leeds, UK.

Topics will Include:
- High Resolution Studies (Both Frequency and Time Resolved) of Molecular Photodissociation or Photoinitiated Processes
- Control of Reactivity via Collision Energy, Selective Vibration of Reagents, or Reagent Alignment
- Demonstrations of Active or Coherent Control of Chemical Processes

Information: http://www.chem.leeds.ac.uk/faraday 113/

JULY 5-9, 1999

*6th INTERNATIONAL SYMPOSIUM ON FIRE SAFETY SCIENCE*
Poitiers, France.

Topics will Include:
- Fire Physics
- Fire Chemistry
- Smoke and Toxic Hazard
- Fire Behavior of Materials
- Stochastic Modeling and Risk Assessment
- Human Behavior and Egress
- Fire Spread
- External Fires
- Structural Behavior
- Fire Detection and Suppression
- Advanced Applications of Fire Safety Science
- Specialized topics in Fire Safety and Protection

Information: 6th IAFSS Symposium Organizers, LCD-ENSMA, Teleport 2, B.P. 109-86960 Futuroscope Cedex, France, 33(0)5 49 49 82 90, Fax 33(0)5 49 49 82 91, e-mail: iafss6@lcd.ensma.fr

♦ JULY 11-16, 1999

*GORDON RESEARCH CONFERENCE ON THE CHEMISTRY AND PHYSICS OF THE DYNAMICS OF SIMPLE SYSTEMS*
Salve Regina University, Newport RI.

Organizing Chairman: C. Chandler
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

♦ JULY 11-16, 1999

*GORDON RESEARCH CONFERENCE ON FREE RADICAL REACTIONS*
Holderness School, Plymouth NH.

Organizing Chairman: D.P. Curran
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

♦ JULY 11-16, 1999

*GORDON RESEARCH CONFERENCE ON THE PHYSICS AND CHEMISTRY OF MATRIX ISOLATED SPECIES*
Plymouth State College, Plymouth NH.

Organizing Chairman: B. Ault
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

♦ JULY 12-15, 1999

*CLEAN AIR V: 5th INTERNATIONAL CONFERENCE ON TECHNOLOGIES AND COMBUSTION FOR A CLEAN ENVIRONMENT*
Lisbon, Portugal.

Information: Maria da Graca Carvalho, Mechanical Engineering Department, Instituto Superior Tecnico, Av Rovisco Pais, 1096 Lisbon Codex, Portugal, 351 (1) 841 7372 or 7186, Fax 351 (1) 847 5545 or (1) 726 2633, e-mail: cleanair@esoterica.pt

JULY 12-16, 1999

*24th INTERNATIONAL CONFERENCE ON PHENOMENA IN IONIZED GASES*
Warsaw, Poland.

Information: J. Wolowski, Institute of Plasma Physics and Laser Microfusion, 23 Hery St., P.O. Box 49, 00-908 Warsaw, Poland, e-mail: icpig99@ifpilm.waw.pl

JULY 18-23, 1999

*THE 1999 DYNAMICS OF MOLECULAR COLLISIONS CONFERENCE*
Lake Harmony PA.

Information: J.J. Valentini, Department of Chemistry, Columbia University, New York, NY 10027, (212) 854-7590, e-mail: Bitnet,VA1Valentini@cuchem

♦ JULY 18-23, 1999

*GORDON RESEARCH CONFERENCE ON ENERGETIC MATERIALS*
Queen's College, Oxford UK.

Organizing Chairman: P.J. Haskins
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

♦ JULY 18-23, 1999

*GORDON RESEARCH CONFERENCE ON PHOTOIONS, PHOTOIONIZATION AND PHOTODETACHMENT*
Plymouth State College, Plymouth NH.

Organizing Chairman: E. Poliakoff
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

JULY 18-23, 1999

*SPIE ANNUAL MEETING*
Denver CO.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

JULY 18-23, 1999

*ASME/JSME FLUIDS ENGINEERING CONFERENCE*
San Francisco CA.

Symposium Programs Include:
- Industrial Applications of Swirling Flows, Organizer, M. Padmanabhan, Alden Research Laboratory, 30 Shrewsbury St., Holden, MA 01520, (508) 829-6000, Fax (508) 829-5939, e-mail: Padu@aldenlab.com
- Numerical Developments in CFD, Organizer, M. Dhaubhadel, Ford Motor Company, (313) 248-5501, (313) 322-1733, e-mail: Mdhaubha@ford.com
- 8th International Symposium on Gas/Particle Flows, Organizer, D. Stock, Washington State University, Pullman, WA 99164, (509) 335-3223, Fax (509) 335-4662, e-mail: stock@mme.wsu.edu

- Turbulent Mixing and Diffusion, Organizers, J.C. Hill, Iowa State University, and K. Ghia, University of Cincinnati.
- Thermal Anemometry, Organizers, J. Foss, Michigan State University, East Lansing, MI 48824, (517) 355-3337, Fax (517) 353-5547, e-mail: Foss@msu.egr, or O.F. Turan, e-mail: Ofturan@dingo.vut.edu.au
- Experimental and Numerical Flow Visualization and Laser Anemometry, Organizer, B. Kahlighi, GM Research & Development, Warren, MI 48090, (810) 986-0885, Fax (810) 986-0918, e-mail: Bkhaligh@cmsa.grm.com
- Finite Element Applications in Fluid Mechanics, Organizer, M. Dhaubhadel, Ford Motor Company, 2000 Rotunda Dr., Dearborn, MI 48121, (313) 248-5501, Fax (313) 322-1733, e-mail: Mdhaubha@ford.com
- Shock Waves and Compressible Flows, Organizers, M. Morris, Bradley University, O. Baysal, Old Dominion University, and A. Kuhl, Lawrence Livermore.
- Optical Methods and Image Processing in Fluid Mechanics, Organizer, R.J. Adrian, University of Illinois, Department of Theoretical and Applied Mechanics, University of Illinois, 216 Talbot Laboratory, 104 S. Wright St., Urbana, IL 61801, (217) 333-1793, Fax (217) 244-5707, e-mail: r-adrian@uiuc.edu

♦ JULY 22-27, 1999

*21st INTERNATIONAL CONFERENCE ON THE PHYSICS OF ELECTRONIC AND ATOMIC COLLISIONS, ICPEAC '99*
Sendai, Japan.

Information: M. Matsuzawa, Applied Physics and Chemistry, University of Electro-Communications, Tokyo, 182-8585, Japan, e-mail: michio@pc.uec.ac.jp, http://power1.pc.uec.ac.jp/sendai

♦ JULY 25-30, 1999

*INTERNATIONAL CONFERENCE ON ANALYTICAL CHEMISTRY: ANALYTICAL SCIENCE IN THE NEXT MILLENNIUM*
Dublin, Ireland.

Information: R. Smyth, Dublin City University, Dublin 9, Ireland, (353) 1-7045-308, Fax (353) 1-7045-032, e-mail: smythm@ccmail.dcu.ie

JULY 25-30, 1999

*17th INTERNATIONAL COLLOQUIUM ON THE DYNAMICS OF EXPLOSIONS AND REACTIVE SYSTEMS*
Heidelberg, Germany.

Information: U. Riedel, Universitat Heidelberg, IWR, Im Neuenheimer Feld 368, D-69120 Heidelberg, Germany, 49(6221) 54 8887, Fax 49(6221) 54 8884, e-mail: icders99@iwr.uni-heidelberg.de, http://reaflow.iwr.uni-heidelberg.de/icders99.html
Deadline: Camera ready Extended Abstracts (up to 4-Pages) of Papers or Posters by December 1, 1998. Electronic Submission is Encouraged, and should be Addressed to: J. Buckmaster, 321A Talbot Laboratory, 104 S. Wright St., Urbana, IL 61801, (217) 333 1803, Fax (217) 244 0720, e-mail: icders@uiuc.edu

♦ JULY 25-30, 1999

*GORDON RESEARCH CONFERENCE ON NONLINEAR OPTICS AND LASERS*
Colby-Sawyer College, New London NH.

Organizing Chairman: A. Weiner
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

AUGUST 1-5, 1999

*16th INTERNATIONAL SYMPOSIUM ON COMBUSTION PROCESSES*
Kazimierz Dolny, Poland.

Topics will Include:
- Combustion in IC Engines
- Combustion Generated Pollutants
- Combustion Diagnostics
- Combustion Chemistry and Physics
- Flames and Detonations
- Fires and Explosions
- Heterogeneous Combustion
- Practical Combustion Systems
- Mathematical Modeling in Combustion

Information: A. Kowalewicz, Radom Technical University, Institute of Maintenance of Vehicles and Machines, Al. Chrobrego 45, 26-600 Radom, Poland, Fax (48)48 440 74, e-mail: kowala@kiux.man.radom.pl
Deadline: 2 Copies of a 1-Page Abstract Due January 31, 1999.

♦ AUGUST 1-5, 1999

*34th INTERSOCIETY ENERGY CONVERSION ENGINEERING CONFERENCE*
Vancouver, British Columbia, Canada.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

AUGUST 1-6, 1999

*5th WORLD CONGRESS OF THEORETICALLY ORIENTED CHEMISTS*
London, UK.

Information: J. Gibson, WATOC '99, The Royal Society of Chemistry, Burlington House, London W1V 0BN, UK, (171) 437 8656, Fax (171) 734 1227, e-mail: conferences@rsc.org

♦ AUGUST 1-6, 1999

*GORDON RESEARCH CONFERENCE ON QUANTUM CONTROL OF ATOMIC AND MOLECULAR MOTION*
Plymouth State College, Plymouth NH.

Organizing Chairmen: R.J. Gordon and P. Brumer
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

♦ AUGUST 8-13, 1999

*GORDON RESEARCH CONFERENCE ON DYNAMICS AT SURFACES*
Proctor Academy, Andover NH.

Organizing Chairman: A. Kleyn
Information: Gordon Research Center, University of Rhode Island, P.O. Box 984, West Kingston, RI 02892, (401) 783-4011, Fax (401) 783-7644, e-mail: grc@grcmail.grc.uri.edu, http://www.grc.uri.edu

AUGUST 14-17, 1999

*33rd ASME NATIONAL HEAT TRANSFER CONFERENCE*
Albuquerque NM.

This Conference will Include a Symposium on Heat Transfer in Combustion and Fire. Topics will Include:
- Radiation and Heat Transfer
- Fundamentals of Combustion
- Practical Combustion
- Combustion Instrumentation and Diagnostics
- Open Forum on Combustion
- Definition of a Model Problem for Experiments and Digital Computing of Fires

Information: M. di Marzo, Mechanical Engineering Department, University of Maryland-College Park, MD, 20742, (301) 405-5257, Fax (301) 314-9477, e-mail: marino@eng.umd.edu, http://www.asme.org/conf/

♦ AUGUST 14-19, 1999

*IUPAC CONGRESS ON FRONTIERS IN CHEMISTRY*
Berlin, Germany.

Information: Gesellschaft Deutscher Chemiker GDCh, P.O. Box 90 04 40, D-60444, Frankfurt am Main, Germany, 49 69 7917 358/360/366, Fax 49 69 7917 475, e-mail: tg@gdch.de

♦ AUGUST 15-20, 1999

*25th INTERNATIONAL SYMPOSIUM ON FREE RADICALS*
Flagstaff AZ.

Information: T.A. Miller, The Ohio State University, Web Site: http://frs.mps.ohio-state.edu/frs

AUGUST 16-19, 1999

*5th INTERNATIONAL SYMPOSIUM ON SELF-PROPAGATING HIGH TEMPERATURE SYNTHESIS*
Moscow, Russia.

Information: Organizing Committee, Institute of Structural Macrokinetics and Materials Science, Russian Academy of Sciences, 7(095)962 80 08, Fax 7(095)962 80 40, e-mail: shs99@ism.ac.ru or merzh@isman0.unicon.msk.su, http://www.ism.ac.ru/SHS99.html

AUGUST 18-21, 1999

*1st INTERNATIONAL CONFERENCE ON ENGINEERING THERMOPHYSICS*
Beijing, China.

Topics will Include:
- Advanced Thermodynamic Cycles and New Energy Systems
- Aerothermodynamics in Turbomachinery and Other Internal Flow Devices
- Heat and Mass Transfer and Heat Exchangers
- Combustion
- Multiphase Flow Problems
- Thermophysics Measurements
- Environmental Problems Related with Thermophsics
- All Other Related Topics

Information: Ms. H. Ke, Chinese Society of Engineering Thermophysics, P.O. Box 2706, Beijing 100080, China, (8610) 62566816, Fax (8610) 62555581, e-mail: xjz@etpserver.etp.ac.cn

♦ AUGUST 22-26, 1999

*218th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
New Orleans LA.

Division of Fuel Chemistry:
- Tutorial on Advanced Analytical Methods for Fossil Fuels and Products
  R.E. Winans, Chemistry Division, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439, e-mail: rewinans@anl.gov
- Molecular and Network Structures of Coal
  M. Iino, Institute of Chemical Reaction Science, Tohoku University, Katahira 2-1-1 Aoba-Ku, Sendai 980, Sendai, Japan, e-mail: iino@icrs.tohoku.ac.jp; R.E. Winans, Chemistry Division, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439, e-mail: rewinans@anl.gov
- Hydrogen Production, Storage, and Utilization
  C. Gregoire-Padro, National Renewable Energy Laboratory, 1617 Cole Boulevard, Golden, CO 80401, (303) 275-2919.

- Chemistry of Reactive Intermediates and Modeling in Hydrocarbon Conversion
  J.A. Franz, M.T. Klein, Rutgers, State University of New Jersey, College of Engineering, Office of the Dean, 98 Brett Road, Piscataway, NJ 08854, (732) 445-2214, Fax (732) 445-5313, e-mail: mtklein@email.eng.rutgers.edu
- Recent Advances in Fuel Cells
  M.A. Wojtowicz, Advanced Fuel Research Inc., 87 Church Street, East Hartford, CT 06108, (860) 528-9806 ext. 142, Fax (860) 528-0648, e-mail: marek@afrinc.com

Division of Physical Chemistry:

- Imaging in Chemical Dynamics
  A. Suits, Department of Chemistry, University of California, Berkeley, CA 94720, (510) 486-4754, Fax (510) 486-5311, e-mail: agsuits@lbl.gov; R. Continetti, Department of Chemistry and Biochemistry, University of California, 9500 Gilman Drive, La Jolla, CA 92093-0314, (619) 534-5999, Fax (619) 534-7042, e-mail: rcontinetti@ucsd.edu
- Electronically Nonadiabatic Processes in Gaseous, Cluster, and Condensed Media
  L.J. Butler, Department of Chemistry, University of Chicago, 5640 S Ellis Avenue, Chicago, IL 60637, (773) 702-7206, Fax (773) 702-5863, e-mail: ljb4@midway.uchicago.edu; D.G. Truhlar, Department of Chemistry, University of Minnesota, Minneapolis, MN 55455, (612) 624-7555, Fax (612) 626-9390, e-mail: truhlar@umn.edu
- Water Clusters, Liquid Water, and Ice: Water in Biological Systems & Heterogeneous Atmospheric Processes
  M. Johnson, Department of Chemistry, Yale University, 225 Prospect Street, New Haven, CT 06520, (203) 432-3916, Fax (203) 432-6144, e-mail: johnson@cluster.chem.yale.edu; R. Saykally, Department of Chemistry, University of California, Berkeley CA 94720, (510) 642-8269, Fax (510) 642-8369, e-mail: saykally@cchem.berkeley.edu
- Chemical Waves, Fronts and Patterns
  J. Pojman, Department of Chemistry and Biochemistry, University of Southern Mississippi, Hattiesburg, MS 39406, (601) 266-5035, Fax (601) 266-6075, e-mail: john.pojman@usm.edu; I. Epstein, Department of Chemistry, Brandeis University, Mail stop 134, Waltham, MA 02254, (781) 736-2101, Fax (781) 736-3457, e-mail: epstein2@binah.cc.brandeis.edu; V. Volpert, Laboratoire d'analyse numirique, University Lyon I, Batiment 101, 43, bd du 11 Novembre 1918, 69622 Villeubanne Cedex, France, 33-472-448317, Fax 33-472-448053, e-mail: volpert@lan1.univ-lyon1.fr

Deadline: Four Copies of Abstract (Original on ACS Abstract Form) Due to Symposium Chair by March 15, 1999. Preprints are Due by April 15, 1999.

AUGUST 22-26, 1999

*14th OZONE WORLD CONGRESS*
Dearborn MI.

Information: M. Istok, IOA/PAG Executive Director, 31 Strawberry Hill Avenue, Stamford, CT 06902, (203) 348-3542, Fax (203) 967-4845, e-mail: mistok@i-2000.com, or mistok@int-ozone-assoc.org

AUGUST 23-27, 1999

*12th INTERNATIONAL CONFERENCE ON FOURIER TRANSFORM SPECTROSCOPY*
Waseda University, Tokyo, Japan.

Information: ICOFTS-12 Conference Office, c/o Koichi Itoh, General Chairman, Department of Chemistry, School of Science and Engineering, Waseda University, Shinjuku-ku, Tokyo 169, Japan, http://www.chem.waseda.ac.jp/icofts/

♦ AUGUST 29-SEPTEMBER 3, 1999

*ENGINEERING FOUNDATION CONFERENCE ON ENVIRONMENTAL TECHNOLOGY FOR OIL POLLUTION: REMEDIATION AND POLLUTION PREVENTION*
Jurata, Poland.

Organizing Chairmen: J. Hupka and J. Miller
Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441.

SEPTEMBER 5-9, 1999

*15th EUROPEAN CONFERENCE ON THERMOPHYSICAL PROPERTIES*
Wurzburg, Germany.

Information: J. Fricke, Physikalisches Institut der Universitat, Am Hubland, D-97074 Wurzburg, Germany, e-mail: ectp@zae.uni-wuerzburg.de

SEPTEMBER 12-15, 1999

*1st INTERNATIONAL SYMPOSIUM ON TURBULENCE AND SHEAR FLOW PHENOMENA*
Santa Barbara CA.

Information: S. Banerjee, Department of Chemical Engineering, University of California at Santa Barbara, Santa Barbara, CA 93106, (805) 893 3456, Fax (805) 893 4731, e-mail: tsfp@engineering.ucsb.edu

♦ SEPTEMBER 12-15, 1999

*6th INTERNATIONAL CONFERENCE ON METHODS AND APPLICATIONS OF FLUORESCENCE SPECTROSCOPY*
Paris, France.

Information: B. Valeur, MAFS6-Conservatoire National des Arts et Metiers, 292 rue Saint-Martin, F-75141 Paris Cedex 03, France, 33 01 40 27 23 89, Fax 33 01 40 27 23 62, e-mail: mafs6@cnam.fr, http://www.lbpa.ens-cachan.fr/photobm/mafs6

♦ SEPTEMBER 12-17, 1999

*10th INTERNATIONAL CONFERENCE ON COAL SCIENCES: PROSPECT FOR COAL SCIENCE IN THE 21ST CENTURY*
Taiyuan, Shanxi

Topics will Include:
- Fundamentals and General Aspects
- Combustion and Conversion Science
- Chemicals and Materials from Coal
- Coal Preparation and Beneficiation
- Environment Aspects

Information: L. Zhou, 10th ICCS Secretariat, Institute of Coal Chemistry, Chinese Academy of Sciences, P.O. Box 165, Tiayuan, Shanxi, 030001, P.R. China, Phone/Fax (86) 351-4048967, e-mail: iccs99@ms.sxicc.ac.cn, http://www.sxicc.ac.cn

SEPTEMBER 17-22, 1999

*PHOTONICS EAST*
Boston MA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

♦ SEPTEMBER 19-24, 1999

*ENGINEERING FOUNDATION CONFERENCE ON MICROGRAVITY FLUID PHYSICS AND HEAT TRANSFER*
Oahu HI.

Organizing Chairpersons: V. Dhir, J. Straub and Y. Fujita
Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441.

♦ SEPTEMBER 19-24, 1999

*5th ENGINEERING FOUNDATION CONFERENCE ON THE CONTROL OF PARTICULATE PROCESSES*
Queensland, Australia.

Organizing Chairman: J. Litster
Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441.

SEPTEMBER 25-OCTOBER 1, 1999

*INTERDISCIPLINARY LASER SCIENCE CONFERENCE AND THE ANNUAL MEETING OF THE OPTICAL SOCIETY OF AMERICA*
Santa Clara CA.

Information: Meetings Department, Optical Society of America, 201 Massachusetts Avenue, Washington, DC 20036, (202) 223-8130.

♦ OCTOBER 4-8, 1999

*FULLERENES AND ATOMIC CLUSTERS*
St. Petersburg, Russia.

Information: e-mail: fuller@vul.ioffe.rssi.ru, Web Site: http://www.ioffe.rssi.ru/IWFAC99/index.html

♦ OCTOBER 5-8, 1999

*GASEOUS ELECTRONICS CONFERENCE*
Norfolk VA.

Information: L. Vuskovic, Old Dominion University, e-mail: lxv100f@oduvm.cc.odu.edu

OCTOBER 6-9, 1999

*35th WESTERN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
Ontario CA.

Information: V.L. Barrett, Sunkist Growers, 760 East Sunkist Street, Ontario, CA 91761, (909) 933 2291, Fax (909) 933 2453, e-mail: vbarrett@isdnt.sunkist-ppd.com

OCTOBER 17-20, 1999

*51st SOUTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
Knoxville TN.

Information: C. Feigerle, University of Tennessee, Department of Chemistry, Knoxville, TN 37996, (615) 974-2129, e-mail: reglmtgs@acs.org

OCTOBER 17-22, 1999

*JOINT INTERNATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY*
Honolulu HI.

Topics will Include:
- Corrosion
- Plasma Etching Processes
- Diamond Formation and Materials
- Fullerenes
- Fuel Cells

Information: http://www.electrochem.org/meetings
Deadline: Abstracts Due by May 14, 1999.

OCTOBER 21-23, 1999

*JOINT 55th SOUTHWEST/15th ROCKY MOUNTAIN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
El Paso, TX.

Information: K. Pannell, Chemistry Department, University of Texas, El Paso, TX 79968, (915) 747 5796, Fax (915) 747 5748 e-mail: kpannel@utep.edu

♦ OCTOBER 24-27, 1999

*FIRE RETARDANT CHEMICAL ASSOCIATION MEETING*
New Orleans LA.

Information: FRCA, 851 New Holland Avenue, P.O. Box 3535, Lancaster, PA 17604, (717) 219-5616.

♦ OCTOBER 24-28, 1999

*6th ENGINEERING FOUNDATION CONFERENCE ON THE PRESENT AND FUTURE ENGINES FOR AUTOMOBILES*
Orvieto, Italy.

Organizing Chairman: R. Rinolfi, T. Kamimoto and D. Foster
Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441.

OCTOBER 24-29, 1999

*26th ANNUAL CONFERENCE OF THE FEDERATION OF ANALYTICAL CHEMISTRY AND SPECTROSCOPY SOCIETIES*
Vancouver, British Columbia, Canada.

Information: Division of Analytical Chemistry, FACSS, (505) 820-1648, Fax (505) 989-1073, http://FACSS.org/info.html

♦ OCTOBER 25-28, 1999

*INTERNATIONAL FUEL AND LUBRICANTS FALL MEETING AND EXPOSITION OF THE SOCIETY OF AUTOMOTIVE ENGINEERS*
Toronto, Ontario, Canada.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

OCTOBER 27-29, 1999

*34th MIDWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
Quincy IL.

Information: H.D. Wohlers, Truman State University, Science Hall, 100 East Normal, Kirksville, MO63501, (816) 785 4625, Fax (816) 785 4045, e-mail: wohlers@truman.edu

♦ NOVEMBER 7-9, 1999

*SOUTHEASTERN SECTION MEETING OF THE AMERICAN PHYSICAL SOCIETY*
Chapel Hill NC.

Information: T. Clegg, e-mail: clegg@TUNL.tunl.DUKE.edu, or the American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ NOVEMBER 14-19, 1999

*1999 ASME INTERNATIONAL MECHANICAL ENGINEERING CONGRESS AND EXPOSITION: SYMPOSIUM ON FIRE AND COMBUSTION SYSTEMS*
Nashville TN.

Topics will Include:

- Combustion in Practical Systems
- Turbulence/Radiation Interactions
- Generation of Soot and Species
- Microgravity Combustion
- Droplet and Spray Combustion
- Fire Growth and Suppression
- Diagnostic Developments for Fire and Combustion Systems
- Combustion Synthesis of Materials

Information: W. Gill, STS Certification Environments, P.O. Box 5800, Mail Stop 0853, Sandia National Laboratories, Albuquerque, NM 87185, (505) 845-3193, Fax (505) 844-0078, e-mail: wgill@sandia.gov, Web site: http://www.asme.org/conf/congress99/
Deadline: Abstracts Due by January 29, 1999

NOVEMBER 14-19, 1999

*EASTERN ANALYTICAL SYMPOSIUM*
Somerset NJ.

Information: S. Gold, Eastern Analytical Symposium, P.O. Box 633, Montchanin, DE 19710, (302) 738-6218, Fax (302) 738-5275, http://www.eas.org

NOVEMBER 14-19, 1999

*ASME INTERNATIONAL MECHANICAL ENGINEERING CONGRESS AND EXPOSITION*
Nashville TN.

Information: P. Pfund, Conference Chair, Babcock and Wilcox, 1562 Beeson Street, Alliance, OH 44601, e-mail: phil.a.pfund@mcdermott.com

NOVEMBER 21-23, 1999

*52nd MEETING OF THE AMERICAN PHYSICAL SOCIETY, DIVISION OF FLUID DYNAMICS*
New Orleans LA.

Information: M. Gad-el-Hak, Department of Aerospace and Mechanical Engineering, University of Notre Dame, Notre Dame, IN 46556, e-mail: mohamed.gad-el-hak.1@nd.edu

♦ NOVEMBER 29-30, 1999

*SPQ-99/EUROPE: SPECTROSCOPY IN PROCESS AND QUALITY CONTROL*
London, UK.

Information: S. Roberts, Advanstar Communications, Advanstar House, Sealand Road, Chester CH1 4RN, UK, (44) 1244 378 888, Fax: (44) 1244 370 011, e-mail: sroberts@advanstar.com

DECEMBER 7-9, 1999

*8th INDIAN SOCIETY FOR MASS SPECTROMETRY SYMPOSIUM*
Hyderabad, India.

Information: S.K. Aggarwal, Secretary, ISMAS and Head, Mass Spectrometry Section, Fuel Chemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400 085, India, Fax (91) 22-556-0750, e-mail: skaggr@magnum.barc.ernet.in

♦ JANUARY 10-15, 2000

*WINTER CONFERENCE ON PLASMA SPECTROCHEM*
Fort Lauderdale FL.

Information: R. Barnes, ICP Info Newsletter, P.O. Box 666, Hadley, MA 01003, e-mail: winterconf@chem.umass.edu

♦ JANUARY 22-28, 2000

*PHOTONICS WEST*
San Jose CA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

♦ MARCH 6-9, 2000

*SAE INTERNATIONAL CONGRESS AND EXPOSITION*
Detroit MI.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

♦ MARCH 20-24, 2000

*MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY*
Minneapolis MN.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ MARCH 26-31, 2000

*219th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
San Francisco CA.

Division of Fuel Science:
- Fuel Science in the Year 2000: Where Do We Stand, Where Do We Go From Here?
  G.P. Huffman, 533 S. Limestone Street, Suite 111, University of Kentucky, Lexington, KY 40506-0043, (606) 257-4027, Fax (606) 257-7215 e-mail: cffls@pop.uky.edu

- Advances in F-T Chemistry
  B.H. Davis, Center for Applied Energy Research, University of Kentucky, Lexington, KY 40511, (606) 257-0251, Fax (606) 257-0302, e-mail: davis@alpha.caer.uky.edu
- Molecular Modeling of Solid-Fuel Reactions
  L.R. Radovic, Fuel Science Program, Pennsylvania State University, 217 Academic Projects Building, University Park, PA 16802, (814) 863-0594, Fax (814) 865-3075, e-mail: lrr3@psu.edu
- Applications of X-ray and Gamma Ray Techniques in Fuel Science
  K.A. Carrado, CHM/200, 9700 S. Cass Avenue, Argonne National Laboratory, Argonne, IL 60439-4831, (630) 252-7968, Fax (630) 252-9288, e-mail: kcarrado@anl.gov

Division of Petroleum Chemistry:

- New Chemistry of Fuel Additives
  D. Daly, Fuel Products, Strategic Technology, Lubrizol Co., 29400 Lakeland Blvd., Wickliffe, OH 44092, (440) 943-1200 ext. 4261, Fax (440) 943-9022, e-mail: dtd@lubrizol.com
- $CO_2$ Conversion and Utilization in Refinery and Chemical Processing
  C. Song, Pennsylvania State University, 209 Academic Projects Building, University Park, PA 16802, (814) 863-4466, Fax (814) 865-3075, e-mail: csong@psu.edu; A.M. Gaffney, DuPont Central R&D, Experimental Station, P.O. Box 80262, Wilmington, DE 19880, (302) 695-1800, Fax (302) 695-8347, e-mail: anne.m.gaffney@usa.dupont.com

Division of Physical Chemistry:

- Physical Chemistry at High Pressure and Temperature
  A.P. Alivisatos, Department of Chemistry, University of California, Berkeley CA 94720, (510) 643-7371, Fax (510) 642-6911, e-mail: alivis@uclink4.berkeley.edu; R. Jeanloz, Department of Geology & Geophysics, University of California, Berkeley CA 94720, (510) 642-2639, Fax (510) 643-9980, e-mail: jeanloz@uclink.berkeley.edu
- Atmospheric Chemistry (Harold Johnston Festschrift)
  C.E. Miller, Department of Chemistry, Haverford College, Haverford, PA 19041, (610) 896-1388, Fax (610) 896-4904, e-mail: cmiller@haverford.edu

Information: From the Individual Chairpersons or from Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

Deadline: 4 Copies of 150-Word Abstract (Original on ACS Abstract Form to Symposium Organizer by August 1, 1999.

♦ MARCH 26-31, 2000

*CORROSION/2000*
Orlando FL.

Information: NACE Headquarters, Meetings Department, P.O. Box 218340, Houston, TX 77218, (281) 228-6200, Fax (281) 228-6300, http://www.nace.org

MAY 7-12, 2000

*CLEO/QELS 2000*
San Francisco CA.

Information: Meetings Department, American Physical Society, One Physics Ellipse, College Park, MD 20740, (301) 209-3286, http://www.osa.org/mtg_conf, http://physics.wm.edu/~cooke/dis/dis.html

♦ MAY 14-19, 2000

*197th MEETING OF THE ELECTROCHEMICAL SOCIETY*
Toronto, Ontario, Canada.

Topics Include:
- General Session on Corrosion
- Plasma Processing
- 15th International Conference on Chemical Vapor Deposition
- Sensors for Energy Technologies

Information: http://www.electrochem.org/meetings

♦ MAY 16-19, 2000

*33rd MIDDLE ATLANTIC REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
Newark DE.

Information: G.L. Trainor, DuPont Pharmaceuticals Co., P.O. Box 80353, Wilmington, DE 19880, (302) 695-3580, Fax (302) 695-8344, e-mail: trainogl@carbon.dmpc.com

♦ MAY 17-19, 2000

*32nd CENTRAL REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
Covington KY.

Information: R. D'Alonzo, Procter & Gamble, Sharon Woods Technical Center, 11450 Grooms Road, Cincinnati, OH 45242, (513) 626-1977, Fax (513) 626-5145, e-mail: dalonzorp@pg.com

♦ JUNE 4-7, 2000

*32nd GREAT LAKES REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
Fargo ND.

Information: G.J. McCarthy, North Dakota State University, Department of Chemistry, Ladd Hall 104B, Fargo, ND 58105, (701) 231-7193, Fax (701) 231-8883, e-mail: gmccarth@prarie.nodak.edu

♦ JUNE 8-10, 2000

*JOINT 55th NORTHWEST/16th ROCKY MOUNTAIN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
Idaho Falls ID.

Information: E.G. Meyer, 214 Arts & Sciences, University of Wyoming, Laramie, WY 82071, (307) 766-5445.

♦ JUNE 18-21, 2000

*29th NORTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
Storrs CT.

Information: G. Epling, University of Connecticut, 215 Glenbrook Road, Storrs, CT 06269, (860) 486-3214, Fax (860) 486-2981, e-mail: epling@nucleus.chem.uconn.edu

♦ JUNE 18-23, 2000

*OPTICS IN COMPUTING*
Quebec City, Quebec, Canada.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

♦ JUNE 19-20, 2000

*CEC/SAE FUELS AND LUBRICANTS SPRING MEETING AND EXPOSITION*
Le Palais des Congress, Paris, France.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

JULY 23-28, 2000

*ENERGEX 2000: 8th INTERNATIONAL ENERGY FORUM*
Las Vegas NV.

Topics will Include:
- Renewable Energies
- Clean Coal Technologies
- Fossil Fuels
- Energy and Economics
- Climatic Change
- International Law
- General Topics
- International Reports
- Nuclear Energy
- Architecture

Information: P. Catania, Faculty of Engineering, University of Regina, Regina, SK S4S 0A2, Canada, (306) 585-4363, Fax (306) 585-4855, e-mail: peter.catania@uregina.ca, http://www2.regina.ism.ca/ief/index/htm or http://www.energysource.com/ief/updates/

♦ JULY 30-AUGUST 4, 2000

*SPIE ANNUAL MEETING*
San Diego CA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

♦ JULY 30-AUGUST 4, 2000

*28th INTERNATIONAL SYMPOSIUM ON COMBUSTION*
Edinburgh, Scotland.

Information: S.S. Terpack, The Combustion Institute, 5001 Baum Boulevard, Suite 635, Pittsburgh, PA 15212, (412) 687-1366, Fax (412) 687-0340, e-mail: combust@telerama.lm.com

♦ AUGUST 20-24, 2000

*220th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
Washington DC.

Division of Fuel Chemistry:
- 1990 Clean Air Act Amendments: A 10-Year Assessment
  J.J. Helble, University of Connecticut, Department of Chemical Engineering, U-222, Storrs, CT 06269, (860) 486-4602, Fax (860) 486-2959, e-mail: helble@eng2.uconn.edu
- Inorganics in Fossil Fuels, Waste Materials, and Biomass: Characterization, Combustion Behavior, and Environmental Issues
  C.L. Senior, Physical Sciences, Inc., 20 New England Business Center, Andover, MA 01810, (978) 689-0003, Fax (978) 689-3232, e-mail: senior@psicorp.com
- Waste Material Recycling for Energy and Other Applications
  S.V. Pisupati, Fuel Science Program, Pennsylvania State University, 404 Academic Projects Building, University Park, PA 16802, (814) 865-0874, Fax (814) 863-8892, e-mail: sxp17@psu.edu
- Fossil Fuels and Global Climate/$CO_2$ Abatement
  R. Warzinski, USDOE/FETC, Box 10940, Building 83-324, Pittsburgh, PA 15236, (412) 892-5863, e-mail: warzinsk@fetc.doe.gov

Division of Petroleum Chemistry:
- Emission Control in Petroleum Processing
  P. O'Connor, U.S. Ozkan, Department of Chemical Engineering, Ohio State University, 140 W. 19th Avenue, Columbus, OH 43210, (614) 292-6623, Fax (614) 292-3769, e-mail: ozkan.1@osu.edu
- Structure of Jet Fuels VI
  W.E. Harrison, Department of the Air Force, WL/POSF, Building 490, Area B, 1790 Loop Road N., Wright-Patterson AFB, OH 45433, (937) 255-6601, Fax (937) 255-1125, e-mail: harriswe@wl.pafb.af.mil

Information: From the Individual Chairpersons or from the Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

♦ AUGUST 22-25, 2000

*9th INTERNATIONAL (MILLENNIUM) SYMPOSIUM ON FLOW VISUALIZATION*
Edinburgh, Scotland.

Information: I. Grant, Heriot-Watt University, Edinburgh, Scotland, EH10 5PJ, UK, (44) 1314478800, Fax (44) 1314478660, e-mail: 9misfv@ode-web.demon.co.uk, Web Site: http://www.ode-web.demon.co.uk/9misfv
Deadline: Abstract Template should be Downloaded from the Web. 4 Pages or Less to be Submitted by December 12, 1999. Final Manuscripts Due May 15, 2000.

♦ SEPTEMBER 10-15, 2000

*CONFERENCE ON LASERS AND ELECTRO-OPTICS (CLEO) AND THE INTERNATIONAL QUANTUM ELECTRONICS CONFERENCE (IQEC)*
Nice, France.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org

♦ SEPTEMBER 19-21, 2000

*THE HYDROGEN ENERGY FORUM 2000*
Munich, Germany.

Information: The Future Energies Forum, "Forum fur Zukunftsenergien", Godesberger Allee 90, D-53175 Bonn, Germany, Fax 49(0) 228-959 56-50, e-mail: energie.forum@t-online.de

♦ SEPTEMBER 22-30, 2000

*27th ANNUAL CONFERENCE OF THE FEDERATION OF ANALYTICAL CHEMISTRY AND SPECTROSCOPY SOCIETIES*
Nashville TN.

Information: Division of Analytical Chemistry, FACSS, (505) 820-1648, Fax (505) 989-1073, Web Site: http://FACSS.org/info.html

♦ OCTOBER 16-19, 2000

*INTERNATIONAL FUEL AND LUBRICANTS FALL MEETING AND EXPOSITION OF THE SOCIETY OF AUTOMOTIVE ENGINEERS*
Baltimore MD.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, Web Site: http://www.sae.org

♦ NOVEMBER 13-18, 2000

*EASTERN ANALYTICAL SYMPOSIUM OF THE AMERICAN CHEMICAL SOCIETY*
Somerset NJ.

Information: S. Gold, Eastern Analytical Symposium, P.O. Box 633, Montchanin, DE 19710, (302) 738-6218, Fax (302) 738-5275, Web Site: http://www.eas.org

♦ DECEMBER 6-8, 2000

*JOINT 52nd SOUTHEAST/56th SOUTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY*
New Orleans LA.

Information: A. Pepperman, SRRC, USDA-ARS, 1100 Robert E. Lee Boulevard, New Orleans, LA 70179, (208) 286-4510, Fax (208) 286-4367, e-mail: abpep@nola.srrc.usda.gov

♦ DECEMBER 14-19, 2000

*INTERNATIONAL CHEMICAL CONGRESS OF PACIFIC BASIN SOCIETIES*
Honolulu HI.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

# CURRENT BIBLIOGRAPHY RELEVANT TO FUNDAMENTAL COMBUSTION

November 1998

Keith Schofield, ChemData Research, P.O. Box 40481
Santa Barbara, CA 93140, (805) 966-7768, Fax (805) 893-8797
e-mail: combust@mrl.ucsb.edu
http://www.ca.sandia.gov/CRF/Publications/CRB/CRB.html

## 1. FUELS/SYNFUELS - GENERAL

78408. Rosen, M.A., and D.S. Scott, "Comparative Efficiency Assessments for a Range of Hydrogen Production Processes," *Int. J. Hydrogen Energy* 23, 653-659 (1998).
$H_2$ Fuel Production Processes Comparative Analysis

78409. Steinberg, M., "Production of Hydrogen and Methanol from Natural Gas with Reduced $CO_2$ Emission," *Int. J. Hydrogen Energy* 23, 419-425 (1998).
$H_2$,$CH_3OH$ Production $CH_4$ Pyrolysis $CO_2/H_2$ Conversion

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$H_2$ Fuel Cryogenic I.C. Engine Usage Feasibility

78411. Contreras, A., S. Yigit, K. Ozay and T.N. Veziroglu, "Hydrogen as Aviation Fuel: A Comparison with Hydrocarbon Fuels," *Int. J. Hydrogen Energy* 22, 1053-1060 (1997).
$H_2$ Fuel Aviation Potential Uses

78412. Pohl, H.W., and V.V. Malychev, "Hydrocarbon in Future Civil Aviation," *Int. J. Hydrogen Energy* 22, 1061-1069 (1997).
$H_2$ Fuel Civil Aviation Potential Uses

78413. Campbell, C.J., and J.H. Laherrere, "The End of Cheap Oil: Global Production of Conventional Oil Will Begin to Decline Sooner than Most People Think, Probably Within 10 Years," *Scientific Am.* 278(3), 78-83 (1998).
Oil Production Reserves Review

78414. George, R.L., "Mining for Oil: More Oil is Trapped in Canadian Sands than Saudi Arabia Holds in Its Reserves. The Technology Now Exists to Exploit This Vast Resource Profitably," *Scientific Am.* 278(3), 84-85 (1998).
Oil Shale Processing Technologies Review

## 2. LIQUEFACTION/GASIFICATION

| | | |
|---|---|---|
| 78415. | Fouda, S.A., "Liquid Fuels from Natural Gas: Natural Gas is Cleaner and More Plentiful Than Oil. New Ways to Convert It to Liquid Form May Soon Make It Just as Cheap and Convenient to Use in Vehicles," *Scientific Am.* 278(3), 92-95 (1998). | Liquefaction<br>Natural Gas<br>Technologies<br>Review |
| 78416. | Periana, R.A., D.J. Taube, S. Gamble, H. Taube, T. Satoh and H. Fujii, "Platinum Catalysts for the High Yield Oxidation of Methane to a Methanol Derivative," *Science* 280, 560-564 (1998). | Liquefaction<br>$CH_4/CH_3OH$<br>Pt Catalysts<br>High Yields |
| 78417. | Dong, Y., and M. Steinberg, "HYNOL: An Economical Process for Methanol Production from Biomass and Natural Gas with Reduced $CO_2$ Emission," *Int. J. Hydrogen Energy* 22, 971-977 (1997). | Liquefaction<br>Biomass<br>$CH_3OH$ Formation<br>Closed Cycle<br>Process |
| (78691) | Biomass/Fossil Fuel Conversion to $CH_3OH$ and C(s), $CO_2$ Mitigation Concept | Liquefaction |
| 78418. | Ramdoss, P.K., and A.R. Tarrer, "High Temperature Liquefaction of Waste Plastics," *Fuel* 77, 293-299 (1998). | Liquefaction<br>Plastic Wastes<br>Gas/Oil Yields |
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Commercial Boilers
Gas, Oil Fired
Heat Transfer
Emissions
1-D Model

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Pulverized Coal
Boiler
Front Wall Fired
Measurements
Emission Levels

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Precessing
Jet Burners
Pulverized Coal
CO,Carbon
Reductions

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Jet Burner
Pulverized Coal
Furnace
Turbulent
Combustion
Modeling

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Incinerator
Traveling Grate
Solid Waste
Model

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Swirl Burner
Low Calorific
Fuels
Axial Piloting
CO,NO
Emissions

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$H_2$ Burner
Coaxial Injector
Swirl
Characterization

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Porous Burners
2 Geometries
2-D Models
Burning Rates

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Porous Burners
$CH_4$/Air
Heat Transfer
CO,NO Emissions
Modeling

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Ceramic Lined Furnaces
Heat Transfer Analysis
Material Optical Property Effects

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Steam Generator
$H_2/O_2$
Spinning Reserve
Automatic Control Method

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Turbines
Direct $H_2$
Burnt Gas Driven Closed Cycle
Efficiency Analysis

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Low $NO_x$ Burner
Performance
Fuel/Oxidant Direct Injection Method

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FBC
Volatiles Combustion
Numerical Model

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FBC
Coal Particle Devolatilization
Heating Rates
Model

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FBC
Coke Particles
Mass Transfer
Bubble Formation
Measurements

(78460) Coal Char Combustion, Kinetic Rates, Pressure Effects

PFBC

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FBC
Biomass Fuels
Fly Ash Formation
Composition

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FBC
Anthracite Coal
2-Stage
Swirl Flow
$CO, NO_x$
Emissions

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FBC
Circulating
Coal/
Wet Sewage Sludge
Co-firing
Emissions

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FBC
Waste Derived
Fuel Testing
Particle
Combustion Times

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FBC
Incineration
Waste Sludge
Ash Formation
Mechanism

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FBC
Solid Fuels
Biomass,Wastes
$O_2$ Sensor
Burn-out Times
Diagnostic

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FBC
Circulating
$CaSO_4$
Dissociation
$SO_2$ Recapture
Conditions

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(See also Section 3 for FBC and Section 21 for Coal Combustion Emissions)

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Lignite Particle
Combustion
Diffusive/Kinetic
Model

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| 78455. | Tunik, Yu.V., "Modeling of Low Speed Combustion of a Methane/Air/ Coal Dust Suspension," *Combust. Expl. Shock Waves, Russia* 33, 431-438 (1997). | Coal Dust/ $CH_4$/Air Combustion Propagation Modeling |
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| (78506) | Devolatilization, IR Pyrometer 2-Color Temperatures | Coal Particle |
| (78420) | Steam Gasification, Kinetic Rates, Reactivities, Mineral Effects | Coal/$CO_2$/$H_2O$ |
| (78419) | Fluidized Bed, Numerical Model | Coal Gasifier |
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Coal, Char Particles
Thermal Conductivity
Photophoretic Measuring Method

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Chars/NO Interactions
CO Effects
Reactivities
Char Source/ Mineral Content Effects

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C(s)/$CO_2$,$H_2O$,$O_2$
Gasification
Surface Dynamic Mechanisms
Energetics

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Hydropyrolysis
Coal/Syngas
Effectiveness

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Coal Pyrolysis
HCN,$NH_3$,$N_2$ Releases
NaOH,KOH,$Ca(OH)_2$ Seeding Effects

(78918) Slow Pyrolysis, Oxidation, HCN, $NH_3$, NO, $N_2O$ Formation, $CaCO_3$ Effects

Petroleum Coke

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Droplet Combustion
Analytical
Simple
Model

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Sprays
Airblast Atomizer
Size Distributions

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Spray
Diffusion Flame
Heat/Mass Transfer
Asymptotic
Numerical Models

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Spray Jets
Penetration
Vaporization
Modeling
Gas/Spray
Comparisons

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Liquid Droplets
Dispersion
Turbulent Mixing
PDA
Sizes,Velocities

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Droplets/Gas
2-Phase
Ignition Delays
Modeling

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$C_2H_5OH$ Spray

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$(CH_3)_2CO$ Droplet
Stream
Interdroplet
Vapor Densities
LIF
Measurements

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Droplet
Fuel Oil
Combustion
Burnout Model
Soot Role

(78586) Continuous Rotating Detonation Wave, Air Mixtures

Kerosene/Diesel
Fuel Sprays

(78454) Slurries, Singlet Droplet Combustion, Efficiencies, Size Effects

Lignite/$H_2O$

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Droplet Combustion
*n*-$C_6H_{14}$/Air
Zone Measurements
Deflectometry

(78510) Doped $C_7H_{16}$, Exciplex LIF Method

Droplet
Temperatures

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Solid Phase
Combustion
Propagation
Heterogeneous
Systems

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| 78482. | Zhu, Y., and S. Yuasa, "Effects of Oxygen Concentration on Combustion of Aluminum in Oxygen/Nitrogen Mixture Streams," *Combust. Flame* 115, 327-334 (1998). | $Al(s)/O_2/N_2$<br>Ignition<br>Temperatures<br>Burning Rates<br>$O_2$ Effects |
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B/Mo
Solid Phase
Combustion
Self-Propagation
Model

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$BaO_2/Cr_2O_3$
Solid Phase
Combustion
Electric Field
Effects

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Solid Phase
Combustion
$La_{0.8}Sr_{0.2}CrO_3$
Synthesis
Temperatures
Optimization

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$Mg/O_2$
$Ti/O_2$
Propagation
Burning Times
Reduced Gravity
Measurements

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$Nb/B/O_2$
$Ti/N_2/O_2$
Two Phase
Combustion
Ignition
Temperature
Variations

78489. Vadchenko, S.G., and A.G. Merzhanov, "Heterogeneous Flame Propagation Model," *Dokl. Phys. Chem.* 352, 40-42 (1997).

$Nb(s)/N_2$
Layered
Thin Plates
Propagation
Model

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Solid Phase
Combustion
Ni/Al;Ti/C
Ni/Al/Ti/B
Propagation
Gravity Effects

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Ni/Al
Ti(s)/Air
Combustion
Propagation
Wave Structure

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Energetic Materials
Porous
Nitramines
Multiphase System
Combustion
Propagation
Model

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HMX,RDX
Pyrolysis
Product Yields
Kinetic
Parameters

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HMX
Propellants
Burning Rate
Predictive Model

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$KNO_3/NaN_3$
Pyrotechnic
$N_2$ Generation
Fire Extinguishers
Role

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PETN
Ignition
Detonation Wave
Induced
Particle Melting

78497. Gongwer, P.E., and T.B. Brill, "Thermal Decomposition of Energetic Materials. 73. The Identity and Temperature Dependence of 'Minor' Products from Flash Heated RDX," *Combust. Flame* 115, 417-423 (1998).

RDX
Flash Pyrolysis
Trace Volatiles
Product FTIR

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TNAZ
Pyrolysis
Unimolecular
Rate Constant
Products
Mechanism
Shock Tube

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Polymer Combustion
Ignition
Retardants
Emissions
Review

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Polyethylene

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PMMA
Cone Heater
Calorimeter
Ignition Times

(78638) Flame Spread, Leading Flame Edge, Fuel Movement Effects
PMMA

(78903) Smoldering Combustion, Propagation, Tomographic Imaging
Polyurethane Foam

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Catalytic Combustion
Lean $CH_4$/Air/Pt
Modeling

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Catalytic
$CH_4/CO+H_2$
Partial Oxidation
FB Reactor
Yields
Model

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Catalytic
Oxidation
CO/NO/Pt
$CO_2$(v) Product Distributions

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Catalytic
Oxidation
$CO/O_2$/Pt
Stochastic Resonance
Behavior

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Catalytic
Oxidation
$CO/O_2$/Pt
Transition State
Energy Barrier
DFT Study

(78654) Catalytic Combustion, Applications, Emissions, Review
I.C. Engines

## 8. MHD

## 9. TEMPERATURES

| | | |
|---|---|---|
| (78456) | Flash Heated Coal Particles, Thermal Delays | Temperature Profiles |
| (78900) | Profiles, NO Saturated LIF, $C_2H_6/O_2/N_2$ Inverse Diffusion Flames | Thermocouple Temperatures |
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| (79102) | Rotational, Vibrational Temperatures, Atomic Electronic Temperatures, Laser Induced Breakdown Plasma, Graphite | CN(B-X) Fe,Pb |
| (78869) | Fe, He, Pb Excitation/OH, $N_2^+$ Rotational Values, He Discharges, Atomic Analysis Detection Limit Media | Temperatures |
| (79091) | Rotational Temperatures, $CH_4/CO_2$ Plasma Discharge | $C_2$(d-a) |
| (78811) | Translational, Vibrational, Rotational Temperatures, He/$N_2$ Discharge, Velocity Modulation Absorption Spectrum | $N_2^+$(A-X) |
| 78510. | Parigger, C., D.H. Plemmons, R.J. Litchford and S.-M. Jeng, "Exciplex Liquid Phase Thermometer Using Time-Resolved Laser Induced Fluorescence," *Opt. Lett.* 23, 76-78 (1998). | Temperatures Exciplex LIF Doped $C_7H_{16}$ Droplets |

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Temperatures
CARS
Spatial
Averaging Effects
Flames

## 10. IGNITION

(78653) Alkane Fuels, I.C. Engine, Kinetic Model, Optimizing Design Tool

Auto-ignition

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Auto-ignition
$n$-$C_4H_{10}$/Air
OH,Temperature
Effects
Ignition Times

78513. Aivazyan, R.G., "Critical Conditions of Self-ignition and Chain Branching Mechanism of Monogermane Oxidation with Oxygen," *Kinet. Catal., Russia* 39, 158-161 (1998).

Self-Ignition
$GeH_4/O_2$
$H_2O_2$ Role
Chain Branching
$CO_2$,$H_2O$
Inhibition

78514. Lee, D., and S. Hochgreb, "Hydrogen Auto-ignition at Pressures Above the Second Explosion Limit (0.6-4.0 MPa)," *Int. J. Chem. Kinet.* 30, 385-406 (1998).

Auto-ignition
$H_2/O_2$
Higher Pressures
$H_2O_2+H$
Rate Constant
Assessment

(78661) Diesel Engine, $H_2$ Fueled, Delay Times, Emissions

Auto-ignition

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Self-ignition
$H_2$/Air
Regimes
Shock Tube
Measurements

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Self-Ignition
$H_2$/Air
Curved Surface
Effects

(78532) Ignition, Combustion Parameters

Gas Cloud
Fireballs

78517. Daou, J., "Ignition and Combustion of Fuel Pockets Moving in an Oxidizing Atmosphere," *Combust. Flame* 115, 383-394 (1998).

Fuel Kernel
Ignition
Combustion
Mechanisms
Model

| | | |
|---|---|---|
| (78471) | Droplets/Gas, 2-Phase, Modeling | Ignition Delays |
| (78637) | Insulation Lagging Material, Fuel Spread, Modeling | Thermal Ignition |
| (78481) | Hydrocarbon Droplet Mixtures, Combustion Modeling | Al(s)/RH<br>Thermal Ignition |
| (78482) | Ignition, Temperatures, Burning Rates, $O_2$ Effects | Al(s)/$O_2$/$N_2$ |
| 78518. | Kim, H.M., H. Enomoto, H. Kato, M. Tsue and M. Kono, "A Study of the Ignition Mechanism of Methane/Air Mixtures by Inert and Catalytic Hot Surfaces," *Combust. Sci. Technol.* 128, 197-213 (1997). | Ignition<br>$CH_4$/Air<br>Inert/Catalytic<br>Hot Surfaces<br>Measurements<br>Model |
| (78527) | Strained $C_3H_8$/Air Interface, Structure, NO, $NO_2$ Formation, Asymptotic Analysis | Ignition Modes |
| (78596) | $C_3H_8$/Air Explosions, Vessel/Duct Interactions, Turbulence | Ignition Site Effects |
| (78914) | Ignition Delays, Shock Tube, Stirred Reactor Mechanisms, Measurements, Kinetic Model | *c*-$C_5H_{10}O/O_2$ |
| (78499) | Ignition, Combustion, Retardants, Emissions, Review | Polymer |
| (78496) | Ignition, Detonation Wave, Induced Particle Melting | PETN |
| (78500) | Ignition Times, Cone Heater Calorimeter | PMMA |
| 78519. | Bui, P.-A., E.A. Wilder, D.G. Vlachos and P.R. Westmoreland, "Hierarchical Reduced Models for Catalytic Combustion: $H_2$/Air Mixtures Near Platinum Surfaces," *Combust. Sci. Technol.* 129, 243-275 (1997). | Catalytic Ignition<br>$H_2$/Air/Pt<br>Reduced Kinetic Schemes |
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| 78521. | Sung, C.J., and C.K. Law, "Ignition of Oscillatory Counterflowing Nonpremixed Hydrogen against Heated Air," *Combust. Sci. Technol.* 129, 347-370 (1997). | Ignition<br>Oscillatory Counterflowing<br>$H_2$/Heated Air<br>Effects<br>Modeling |
| (78458) | Reactivities, Temperature Correlation Assessments | Coal Ignition |

(78457) High Pressures, Temperatures — Coal Particle; Thermal Ignition

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(78477) Solid Combustion, Heating, Model — Microwave Ignition

(78488) Ignition, 2-Phase Combustion, Temperature Variations — Nb/B/$O_2$; Ti/$N_2$/$O_2$

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(78728) Diffusion Flame Structure, Species Profiles, Soot Formation, Flamelet Model — $CH_4$/Air

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| 78531. | Leach, S.V., J.L. Ellzey and O.A. Ezekoye, "A Numerical Study of Reverse Smoldering," *Combust. Sci. Technol.* 130, 247-267 (1997). | Reverse<br>Smoldering<br>Transient Model<br>Reduced Chemistry<br>Quenching |
| (78639) | Reynolds Number Effects, Modeling | Impinging Jet/<br>Wall Flames |
| 78532. | Makhviladze, G.M., J.P. Roberts and S.E. Yakush, "Formation and Combustion of Gas Clouds in Accidental Discharge to the Atmosphere," *Combust. Expl. Shock Waves, Russia* 33, 144-156 (1997). | Gas Cloud<br>Fireballs<br>Ignition<br>Combustion<br>Parameters |

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Triple Flame
Structure
$CH_4$ Jet
PIV Flowfields
OH,$C_2H_n$,LIF
Raman/Rayleigh
Heat Transfer
Role

78534. Kioni, P.N., K.N.C. Bray, D.A. Greenhalgh and B. Rogg, "Experimental and Numerical Studies of a Triple Flame," *Combust. Flame* 116, 192-206 (1999).

Triple Flames
OH,PLIF
PIV Velocities
Measurements
Modeling

78535. Palacios, A., G.H. Gunaratne, M. Gorman and K.A. Robbins, "Karhunen-Loeve Analysis of Spatiotemporal Flame Patterns," *Phys. Rev. E: Statist. Phys., Plasmas, Fluids* 57, 5958-5971 (1998).

Flame Pattern
Video Images
Cellular
Structures
Porous Plug
Burner

78536. Daou, J., and B. Rogg, "Convective Burning of Gaseous Fuel Pockets and Supercritical Droplets," *Combust. Flame* 115, 145-157 (1998).

Cold Fuel Kernel/
Hot Oxidizer
Aerodynamics
Combustion Times

78537. Chen, J.H., T. Echekki and W. Kollmann, "The Mechanism of Two-Dimensional Pocket Formation in Lean Premixed Methane/Air Flames with Implications to Turbulent Combustion," *Combust. Flame* 116, 15-48 (1999).

Unburnt Pocket
Formation
Burn-out
$CH_4$/Air
Vortical Flow
Modeling

78538. Liu, F., and Y. Yoshizawa, "Combustion and Flow of Premixed Lean Hydrogen/Air Mixtures in the Connected Compartments," *Int. J. Hydrogen Energy* 23, 373-379 (1998).

Lean $H_2$/Air
Combustion
Connected
Compartments
Flow Character
Pressure/Time
Histories

78539. Blouquin, R., P. Cambray and G. Joulin, "Radiation-Affected Dynamics of Enclosed Spherical Flames Propagating in Particle Laden Premixtures," *Combust. Sci. Technol.* 128, 231-255 (1997).

Propagation
Spherical Flames
2-Phase
Gas/Particles
Radiation Effects
Modeling

78540. Bychkov, V.V., S.M. Golberg, M.A. Liberman, A.I. Kleev and L.E. Eriksson, "Numerical Simulation of Curved Flames in Cylindrical Tubes," *Combust. Sci. Technol.* 129, 217-242 (1997).

Propagation
Curved Flame Front
Cylindrical Tubes
Velocity/Diameter
Gravity Effects

78541. Rahibe, M., N. Aubry and G.I. Sivashinsky, "Instability of Pole Solutions for Planar Propagating Flames in Sufficiently Large Domains," *Combust. Theory Modeling* 2, 19-41 (1998).

Propagation
Unstable
Planar Flame Fronts
Cusp Modeling

78542. McLaughlin, R.M., and J. Zhu, "The Effect of Finite Front Thickness on the Enhanced Speed of Propagation," *Combust. Sci. Technol.* 129, 89-112 (1997).

Propagation
Shear Layer
Transverse Wind
Thin Reaction Layer
Enhanced Rates
Modeling

78543. Lubkin, G.B., "Combustion in Two Dimensions Yields Fingering Instability," *Phys. Today* 52(1), 19-21 (1999).

2-D Paper
Combustion
Fingering Instabilities
Overview

78544. Mills, K., and M. Matalon, "Burner Generated Spherical Diffusion Flames," *Combust. Sci. Technol.* 129, 295-319 (1997).

Spherical
Diffusion Flames
Microgravity
Stabilities

78545. Atreya, A., and S. Agrawal, "Effect of Radiative Heat Loss on Diffusion Flames in Quiescent Microgravity Atmosphere," *Combust. Flame* 115, 372-382 (1998).

Extinction
Diffusion Flames
Soot Radiative Heat Loss
Role
Modeling

78546. Sohn, C.H., S.H Chung, S.R. Lee and J.S. Kim, "Structure and Acoustic Pressure Response of Hydrogen/Oxygen Diffusion Flames at High Pressure," *Combust. Flame* 115, 299-312 (1998).

Acoustic Instabilities
$H_2/O_2$
Strained Diffusion Flames
High Pressures
Numerical Modeling

78547. Papanikolaou, N., and I. Wierzba, "The Effects of Burner Geometry and Fuel Composition on the Stability of a Jet Diffusion Flame," *J. Energy Resources Technol., Trans. ASME* 119, 265-270 (1997).

Stabilization
Jet Diffusion Flames
Blow-off Limits
Burner, Fuel Effects

78548. Chen, Y.-C., C.-C. Chang, K.-L. Pan and J.-T. Yang, "Flame Lift-off and Stabilization Mechanisms of Nonpremixed Jet Flames on a Bluff Body Burner," *Combust. Flame* 115, 51-65 (1998).

Bluff Body
Stabilization
Flame Modes
Lift-off

78549. Lentati, A.M., and H.K. Chelliah, "Dynamics of Water Droplets in a Counterflow Field and Their Effect on Flame Extinction," *Combust. Flame* 115, 158-179 (1998).

Counterflow
$CH_4$/Air
Water Droplet
Extinction
Modeling

78550. Gol'dshtein, V., I. Goldfarb, I. Shreiber and A. Zinoviev, "Oscillations in a Combustible Gas Bubble," *Combust. Theory Modeling* 2, 1-17 (1998).

Combustible
Gas Bubbles
Oscillations
Numerical
Modeling

(78739) $C_2H_2$ Flames, Acoustic Oscillation Effects

Soot Suppression

78551. Greatrix, D.R., "Structural Vibration and Solid Rocket Combustion Instability," *Can. Aeronaut. Space J.* 44, 9-24 (1998).

Instabilities
Solid Fueled
Rockets
Motor Oscillation
Correlations
Modeling

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Thermoacoustic
Instabilities
Active Control
Modeling

78553. Vanderstraeten, B., D. Tuerlinckx, J. Berghmans, S. Vliegen, E. Van't Oost and B. Smit, "Experimental Study of the Pressure and Temperature Dependence on the Upper Flammability Limit of Methane/Air Mixtures," *J. Hazardous Mat.* 56, 237-246 (1997).

Flammability Limits
$CH_4$/Air
$\leq$55 atm,$\leq$470 K

78554. Karbasi, M., and I. Wierzba, "The Effects of Hydrogen Addition on the Stability Limits of Methane Jet Diffusion Flames," *Int. J. Hydrogen Energy* 23, 123-129 (1998).

Stability Limits
$CH_4$,$H_2$ Jets
Mixture Effects
Blow-out

## 12. TURBULENCE

(See also Section 14 for Turbulent Flowfields)

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Turbulent
Premixed Flames
Scaling Properties
Modeling

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| 78558. | Subramaniam, S., and S.B. Pope, "A Mixing Model for Turbulent Reactive Flows Based on Euclidean Minimum Spanning Trees," *Combust. Flame* 115, 487-514 (1998). | Turbulent<br>Reacting Flows<br>New Mixing Model<br>Performance |
| 78559. | Lee, K.M., and H.D. Shin, "A Large-Scale Structural Mixing Model Applied to Blowout of Turbulent Nonpremixed Jet Flames in a Cross Airflow," *J. Inst. Energy* 70, 128-140 (1997). | Turbulent<br>Jet Flames<br>Cross Airflow<br>Blowout<br>Mixing Model |
| 78560. | Lee, S.-H., I.-S. Jeung and Y. Yoon, "Computational Investigation of Shock-Enhanced Mixing and Combustion," *AIAA J.* 35, 1813-1820 (1997). | Scramjets<br>Shock Enhanced<br>Mixing<br>Combustion Length<br>Turbulence<br>Model |
| 78561. | Raman, G., "Advances in Understanding Supersonic Jet Screech: Review and Perspective," *Prog. Aerospace Sci.* 34, 45-106 (1998). | Supersonic Jet<br>Screech<br>Production Conditions<br>Overview |
| 78562. | Prasad, R.O.S., and J.P. Gore, "An Evaluation of Flame Surface Density Models for Turbulent Premixed Jet Flames," *Combust. Flame* 116, 1-14 (1999). | Turbulent<br>Premixed<br>Jet Flames<br>4 Flame Surface<br>Density Models<br>Evaluated |
| 78563. | Smith, T.M., and S. Menon, "One-Dimensional Simulations of Freely Propagating Turbulent Premixed Flames," *Combust. Sci. Technol.* 128, 99-130 (1997). | Turbulent<br>Premixed Flames<br>Propagation Rates<br>Linear Eddy Model<br>Data Comparisons |
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| 78566. | Gostintsev, Yu.A., A.G. Istratov and V.E. Fortov, "On the Factal Structure of Spherical Flames," *Dokl. Phys. Chem.* 353, 83-84 (1997). | Turbulent<br>Spherical<br>Flames<br>Fractal Structure |
| 78567. | Kratzel, T., E. Pantow and M. Fischer, "On the Transition from a Highly Turbulent Curved Flame into a Tulip Flame," *Int. J. Hydrogen Energy* 23, 45-51 (1998). | Turbulent<br>Curved/<br>Tulip Flame<br>Propagation<br>$H_2$/Air<br>Schlieren |
| 78568. | Arpaci, V.S., and A. Agarwal, "Scaling Laws of Turbulent Ceiling Fires," *Combust. Flame* 116, 84-93 (1999). | Turbulent<br>Buoyancy<br>Driven Flames<br>Ceiling Fire<br>Scaling Laws |
| 78569. | Marracino, B., and D. Lentini, "Radiation Modeling in Non-Luminous Nonpremixed Turbulent Flames," *Combust. Sci. Technol.* 128, 23-48 (1997). | Turbulent Flames<br>Radiative<br>Heat Transfer<br>Non-Luminous<br>Stretched<br>Flamelet Model<br>$CH_4$/Air |
| (78727) | Soot Formation, Thermal Radiation, Measurements | Turbulent<br>$CH_4$/Air Jet |
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| 78571. | Kelman, J.B., and A.R. Masri, "Reaction Zone Structure and Scalar Dissipation Rates in Turbulent Diffusion Flames," *Combust. Sci. Technol.* 129, 17-55 (1997). | Turbulent<br>Diffusion<br>$CH_4$/Air<br>$H_2/CO_2$<br>Structure<br>Scalar<br>Dissipation Rates<br>Rayleigh/Raman<br>LIF,OH |

78572. Jones, W.P., and M. Kakhi, "Application of the Transported PDF Approach to Hydrocarbon/Air Turbulent Jet Diffusion Flames," *Combust. Sci. Technol.* 129, 393-430 (1997).

Turbulent
$CH_4$,$C_3H_8$
Jet Diffusion
Scalar PDF
Predictive Model
Species Densities

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Turbulent
Air Diluted
$CH_4$,$H_2$
Jet Flames
2-D Raman/Rayleigh
Scalar Dissipation

78574. Mansour, M.S., Y.-C. Chen and N. Peters, "Highly Strained Turbulent Rich Methane Flames Stabilized by Hot Combustion Products," *Combust. Flame* 116, 136-153 (1999).

Turbulent
Rich $CH_4$ Flames
Highly Strained
Pilot Stabilized
Raman,Rayleigh
LIPF
Species Profiles
Measurements
Modeling

78575. Jessee, J.P., R.F. Gansman and W.A. Fiveland, "Multi-Dimensional Analysis of Turbulent Natural Gas Flames Using Detailed Chemical Kinetics," *Combust. Sci. Technol.* 129, 113-140 (1997).

Turbulent
Natural Gas
Swirling Flames
Flow/Kinetic
Modeling

78576. Frank, J.H., P.A.M. Kalt and R.W. Bilger, "Measurements of Conditional Velocities in Turbulent Premixed Flames by Simultaneous OH PLIF and PIV," *Combust. Flame* 116, 220-232 (1999).

Turbulent
Natural Gas/Air
2-D PIV
Velocities
PLIF,OH
Measurements

78577. Renfro, M.W., S.D. Pack, G.B. King and N.M. Laurendeau, "Hydroxyl Time-Series Measurements in Laminar and Moderately Turbulent Methane/Air Diffusion Flames," *Combust. Flame* 115, 443-455 (1998).

Turbulent
$CH_4$/Air
OH
ps LIF
Time Resolved

78578. Kok, J.B.W., and J.J.J. Louis, "Modeling Turbulent Combustion in a $CO/H_2$ Diffusion Flame Using Reaction Progress Variables," *Combust. Sci. Technol.* 131, 225-249 (1998).

Turbulent
$CO/H_2$ Diffusion
Flame
Thermal NO
$HO_2$,$H_2O_2$
Intermediates
Effects

78579. Hermanson, J.C., M.B. Colket and J.J. Sangiovanni, "Stability and Emissions of Lean, Turbulent, Premixed Flames with Very Lean Coflow," *AIAA J.* 35, 1705-1711 (1997).

Turbulent
Lean Flames
Stabilization
NO Emissions
Fuel Injection
Strategies

78580. Clemens, N.T., P.H. Paul and M.G. Mungal, "The Structure of OH Fields in High Reynolds Number Turbulent Jet Diffusion Flames," *Combust. Sci. Technol.* 129, 165-184 (1997).

Turbulent
$H_2$/Air
Jet Diffusion
Flames
PLIF,OH
Reynolds
Number Effects

## 13. DETONATIONS/EXPLOSIONS

78581. Montgomery, C.J., A.M. Khokhlov and E.S. Oran, "The Effect of Mixing Irregularities on Mixed-Region Critical Length for Deflagration-to-Detonation Transition," *Combust. Flame* 115, 38-50 (1998).

Deflagration/
Detonation
Transition
Turbulent Mixing
Perturbation
Effects

78582. Gamezo, V.N., D. Desbordes and E.S. Oran, "Formation and Evolution of Two-Dimensional Cellular Detonations," *Combust. Flame* 116, 154-165 (1999).

Detonations
2-D Cellular
Structure
Modeling

78583. Brailovsky, I., and G.I. Sivashinsky, "On Deflagration-to-Detonation Transition," *Combust. Sci. Technol.* 130, 201-231 (1997).

Deflagration/
Detonation
Transition
Tube Flow
Reduced Model

78584. Van Tiggelen, P.J., "Importance of Chemistry in Detonation Waves," *Bull. Soc. Chim. Belg.* 106, 367-370 (1997).

Detonations
CO,$H_2$/$O_2$/Air
Velocities
Halocarbon Effects

78585. Bowen, P.J., D.C. Bull, A. Prothero and J.J. Rowson, "Deflagration of Hydrocarbon Aerosol Fuels," *Combust. Sci. Technol.* 130, 25-47 (1997).

Deflagration
Hydrocarbon/Air
Aerosols
$C_3H_8$,$C_7H_{16}$
Flame Accelerations

78586. Bykovskii, F.A., V.V. Mitrofanov and E.F. Vedernikov, "Continuous Detonation Combustion of Fuel/Air Mixtures," *Combust. Expl. Shock Waves, Russia* 33, 344-353 (1997).

Continuous
Rotating
Detonation Wave
$H_2$,RH/Air
Liquid Spray Fuels

78587. Valishev, A.I., "Calculation of the Detonation Parameters of Acetylene Mixtures," *Combust. Expl. Shock Waves, Russia* 33, 208-210 (1997).

Detonations
$C_2H_2/O_2$,Air
Parameters
Carbon
Condensation Role

78588. Knystautas, R., J.H.S. Lee, J.E. Shepherd and A. Teodorczyk, "Flame Acceleration and Transition to Detonation in Benzene/Air Mixtures," *Combust. Flame* 115, 424-436 (1998).

Detonations
$C_6H_6$/Air
Cell Widths
Kinetic Modeling

78589. Ciccarelli, G., T.G. Ginsberg and J.L. Boccio, "The Influence of Initial Temperature on the Detonability Characteristics of Hydrogen/Air/Steam Mixtures," *Combust. Sci. Technol.* 128, 181-196 (1997).

Detonations
$H_2$/Air/Steam
Cell Size
Dependences

78590. Shebeko, Yu.N., Ya.A. Korolchenko, A.V. Trunev, S.G. Tsarichenko and E.N. Prostov, "The Influence of the Vent Area Location on Hydrocarbon/Air Mixture Deflagration in a Large Scale Vessel," *Combust. Sci. Technol.* 129, 57-69 (1997).

Deflagrations
$H_2$/Air
Large Chamber
Vent Area
Explosive Pressures

78591. Barenblatt, G.I., A.J. Chorin and A. Kast, "The Influence of the Flow of the Reacting Gas on the Conditions for a Thermal Explosion," *Proc. Nat. Acad. Sci. USA* 94, 12762-12764 (1997).

Thermal Explosions
Cylindrical Tube
Flow
Reacting Gases
Critical Values
Modeling

78592. Mol'kov, V.V., V.V. Agafonov and S.V. Aleksandrov, "Deflagration in a Vented Vessel with Internal Obstacles," *Combust. Expl. Shock Waves, Russia* 33, 418-424 (1997).

Explosions
Vented Vessels
Obstacle
Turbulence
Effects
Measurements
Modeling

78593. Wilen, C., A. Rautalin, J. Garcia-Torrent and E. Conde-Lazaro, "Inerting Biomass Dust Explosions under Hyperbaric Working Conditions," *Fuel* 77, 1089-1092 (1998).

Explosions
Biomass Dust
Limiting Oxygen/
Pressure
Relationship

78594. Garcia-Torrent, J., E. Conde-Lazaro, C. Wilen and A. Rautalin, "Biomass Dust Explosibility at Elevated Initial Pressures," *Fuel* 77, 1093-1097 (1998).

Explosions
Biomass Dust
Turbulence
Influence
Measurements

78595. Ponizy, B., and J.C. Leyer, "Flame Dynamics in a Vented Vessel Connected to a Duct. I. Mechanism of Vessel-Duct Interaction," *Combust. Flame* 116, 259-271 (1999).

Explosions
$C_3H_8$/Air
Vessel/Duct
Mutual
Interactions
Measurements

78596. Ponizy, B., and J.C. Leyer, "Flame Dynamics in a Vented Vessel Connected to a Duct. II. Influence of Ignition Site, Membrane Rupture and Turbulence," *Combust. Flame* 116, 272-281 (1999).

Explosions
$C_3H_8$/Air
Vessel/Duct
Interactions
Turbulence
Ignition Site
Effects

## 14. FLOW PHENOMENA/VELOCITIES/DIFFUSION

(See also Section 12 for Turbulent Flowfields and Section 19 for Engine Flowfields)

78597. Snider, R.F., "Relaxation and Transport of Molecular Systems in the Gas Phase," *Int. Rev. Phys. Chem.* 17, 185-225 (1998).

Transport
Relaxation
Properties
Gases
Nonequilibrium
Effects
Review

78598. Stepowski, D., R. Bazile, A. Cessou, P. Colin and S. Guerre, "Laser Diagnostics of Two-Phased Jets in Combustion," *Bull. Soc. Chim. Belg.* 106, 327-330 (1997).

Velocities
Phase Doppler
Raman,LIF
Two Phase Jets
Diagnostics

78599. Francke, E., and J. Amouroux, "Laser Doppler Anemometry (LDA) Simultaneous Measurements of Local Density and Velocity Distribution of Particles in Plasma Fluidized Bed at Atmospheric Pressure," *Plasma Chem. Plasma Process.* 17, 433-452 (1997).

Velocities
Particle
Densities
Plasma
Fluidized Bed
Distributions
LDA

(78470) Dispersion, Turbulent Mixing, PDA, Sizes, Velocities — Liquid Droplets

(78537) Unburnt Pocket Formation, Burn-out, $CH_4$/Air, Modeling — Vortical Flow

(78714) Flowfield, Pulverized Coal Swirl Burner, $NO_x$ Control — Velocities

(78533) Triple Flame Structure, $CH_4$ Jet, OH, $C_2H_n$, LIF, Raman, Rayleigh Scattering, Heat Transfer Role — PIV Flowfields

(78534) Triple Flames, OH, PLIF, Measurements, Modeling — PIV Velocities

| | | |
|---|---|---|
| (78896) | $C_2H_4$ /Air Opposed Jet Flames, Soot Free, Species Profiles, Measurements, Kinetic Model Comparisons | Gas Velocities |
| (79088) | Gas Phase Binary Reactions, Reaction Rates, Diffusion Coefficients, Effects | Nonequilibrium Velocity Distributions |
| (79101) | Laser Ablation, $YBa_2Cu_3O_y$, TOF Mass Analysis | Plume Velocities |
| (78584) | CO, $H_2/O_2$/Ar Mixtures, Halocarbon Effects | Detonation Velocities |
| 78600. | Kwon, O.C., K.T. Aung, L.-K. Tseng, M.A. Ismail and G.M. Faeth, "Comment on 'Approximations for Burning Velocities and Markstein Numbers for Lean Hydrocarbon and Methanol Flames,' by U.C. Muller, M. Bollig and N. Peters," *Combust. Flame* 116, 310-312 (1999). | Burning Velocities $CH_3OH$/Air $C_7H_{16}$,$C_8H_{18}$/Air Calculation Method Comments |
| (78629) | $CH_4$, *n*-$C_7H_{16}$ Flames, Inhibition Effects of $(CF_3)_3N$, $(CF_3)_2NCF_2H$, $(C_2F_5)_2O$, $CF_3SF_5$, $C_2F_5SF_5$ | Burning Velocities |
| 78601. | Aldredge, R.C., V. Vaezi and P.D. Ronney, "Premixed-Flame Propagation in Turbulent Taylor-Couette Flow," *Combust. Flame* 115, 395-405 (1998). | Flame Speeds Turbulent $CH_4$/Air Measurements |
| 78602. | Hassan, M.I., K.T. Aung and G.M. Faeth, "Measured and Predicted Properties of Laminar Premixed Methane/Air Flames at Various Pressures," *Combust. Flame* 115, 539-550 (1998). | Burning Velocities Spherical $CH_4$/Air Flame Stretch Effects |
| 78603. | Bradley, D., R.A. Hicks, M. Lawes, C.G.W. Sheppard and R. Woolley, "The Measurement of Laminar Burning Velocities and Markstein Numbers for *iso*-Octane/Air and *iso*-Octane/*n*-Heptane/Air Mixtures at Elevated Temperatures and Pressures in an Explosion Bomb," *Combust. Flame* 115, 126-144 (1998). | Burning Velocities *i*-$C_8H_{18}$/Air *i*-$C_8H_{18}/C_7H_{16}$/Air Spherical Flame Measurements |
| (78855) | H-Atom Correlation, $Sr^+/SrOH^+$ Ion Measuring Method for H-Atom Concentrations | Burning Velocities |
| (79112) | Diffusion Coefficients, Rg = He,Ne,Ar, P.E. Curve Calculations | $Cl(^2P_{1/2})$/Rg |

## 15. IONIZATION

(See also Section 24 for Cluster Ions, Section 26 for Ion Spectroscopy, Section 40 for Dynamics of Ion-Molecule Reactions, Section 42 for MPI and Laser Ablation Processes, Section 43 for Potential Energy Curves for Ions, Section 44 for Ionic Structures and Section 46 for Thermochemical Values)

| | | |
|---|---|---|
| (79024) | Unimolecular Dissociation, Blackbody Radiative Initiation Evidence | Cluster Ions |

78604. Ye, Y., and R.K. Marcus, "Hardware and Software Systems for the Determination of Charged Particle Parameters in Low Pressure Plasmas Using Impedance-Tuned Langmuir Probes," *Spectrochim. Acta B. At. Spectrosc.* 52, 2025-2041 (1997).

Charged Particle
$e^-$, Ion Densities
Electron Temperature
Energy Distribution
Probe Measurements
Glow Discharge

(78929) Rate Constants, Low Temperatures (1-200 K), Supersonic Flows, Review

$Ar^+ + O_2$
$NO^+(v=1) + M$
$N_2^+ + N_2 + N_2$
$N_2^+ + O_2$
$O_2^+(v=1) + M$

78605. Gonzalez, A.I., D.C. Clary and M. Yanez, "Calculations of Rate Constants for Reactions of First and Second Row Cations," *Theor. Chim. Acta* 98, 33-41 (1997).

$C^+, Si^+, N^+, P^+ + M$
$O^+, S^+, F^+Cl^+ + M$
Rate Constants
$M = CH_2O, CH_3OH, HCOOH, H_2O, H_2S, NH_3$
Calculations

(78975) $C^+(^2P_{1/2,3/2})$ Product Resonances

$CH^+ + h\nu$

(79008) CO(a,X),v, Product Distributions, Calculations

$HCO^+ + e^-$

78606. Talbi, D., and M.C. Bacchus-Montabonel, "Ab Initio Study of a Radiative Association Mechanism Application to the $CH_3^+ + H_2$ Reaction," *Chem. Phys.* 232, 267-273 (1998).

$CH_3^+ + H_2$
Radiative Recombination
P.E. Surface
Rate Constants

(78834) Radiative Lifetime Measurements

$CO^+(X,v)$

78607. Tian, C., and C.R. Vidal, "Electron Impact Dissociative Ionization of Ethane: Cross Sections, Appearance Potentials and Dissociation Pathways," *J. Chem. Phys.* 109, 1704-1712 (1998).

$C_2H_6 + e^-$
17-600 eV
Cross Sections
Channels
Product Ions

78608. McEwan, M.J., G.B.I. Scott and V.G. Anicich, "Ion-Molecule Reactions Relevant to Titan's Ionosphere," *Int. J. Mass Spectrom. Ion Process.* 172, 209-219 (1998).

$C_2N_2^+ + RH$
$C_3H_5^+ + RH, RCN$
$N^+, N_2^+ + RH, RCN$
$Ions + N_2$
Rate Constants
Branching Ratios

78609. Christophorou, L.G., and J.K. Olthoff, "Electron Interactions with $C_3F_8$," *J. Phys. Chem. Ref. Data* 27, 889-913 (1998).

$C_3F_8 + e^-$
Attachment
Cross Sections
Scattering
Review

(78984) Rate Constant, Energy Release, RRKM Model

$C_6H_5Br^+ + h\nu$

| | | |
|---|---|---|
| (78987) | $C_7H_7^+$ Product, Mass Analysis, Rate Constants, Dynamics | $C_6H_5(n\text{-}C_3H_7)^+ + h\nu$ |
| (79004) | IR MPA/MPI, Autoionization Rates, Electronically Excited State Roles | $C_{60}$ |
| 78610. | Lifshitz, C., "Energetics and Dynamics through Time-Resolved Measurements in Mass Spectrometry: Aromatic Hydrocarbons, Polycyclic Aromatic Hydrocarbons and Fullerenes," *Int. Rev. Phys. Chem.* 16, 113-139 (1997). | PAHs,Fullerenes<br>Aromatic HC<br>Photoionization<br>$e^-$ Ionization<br>Ion Fragmentation<br>Efficiencies<br>Isomerization<br>Dissociation<br>Review |
| 78611. | Weilmunster, P., A. Keller and K.-H. Homann, "Large Molecules, Radicals, Ions and Small Soot Particles in Fuel-Rich Hydrocarbon Flames. I. Positive Ions of Polycyclic Aromatic Hydrocarbons (PAH) in Low Pressure Premixed Flames of Acetylene and Oxygen," *Combust. Flame* 116, 62-83 (1999). | PAH Cations<br>$C_2H_2/O_2$<br>Low Pressure<br>Premixed Flames<br>Beam Sampling<br>Mass Analysis |
| (78844) | Oscillator Strengths, 11 Transitions, Measurements | $Co^+$ |
| (78835) | 440 Levels, Radiative Lifetimes, LIF Measurements | $Dy^+$,Dy |
| (78845) | Oscillator Strengths, Transitions, Calculations | $Ge^+$,$As^+$,$Se^+$ |
| (78885) | Photodetachment, Cavity Ringdown Laser Absorption, Density Monitor | $H^-$ |
| (79036) | Isomerization, CO, $CO_2$ Catalyzed Conversion, Collision Energy Effects | $HCN^+/HNC^+$ |
| (79037) | Isomerization, P.E. Surface Fitting | $HOO^-/OOH^-$ |
| 78612. | Anicich, V.G., and A.D. Sen, "Deuterium Exchange in the Systems of $H_2O^+/H_2O$ and $H_3O^+/H_2O$," *Int. J. Mass Spectrom. Ion Process.* 172, 1-14 (1998). | $H_2O^+ + H_2O$<br>$H_3O^+ + H_2O$<br>D-Isotopes<br>Exchange Channels<br>Rate Constants<br>Scrambling |
| 78613. | Mitchell, J.B.A., and C. Rebrion-Rowe, "The Recombination of Electrons with Complex Molecular Ions," *Int. Rev. Phys. Chem.* 16, 201-213 (1997). | $H_3O^+ + e^-$<br>Polyatomic Ions<br>Cluster Ions,$Rg_2^+$<br>Dissociative<br>Recombination<br>Rate Constants<br>Review |
| 78614. | Spanel, P., and D. Smith, "Selected Ion Flow Tube Studies of the Reactions of $H_3O^+$, $NO^+$ and $O_2^+$ with Several Ethers," *Int. J. Mass Spectrom. Ion Process.* 172, 239-247 (1998). | $H_3O^+$ + Ethers<br>$NO^+$,$O_2^+$ + Ethers<br>12 Ethers<br>Rate Constants<br>Product Ions |

78615. Spanel, P., and D. Smith, "Selected Ion Flow Tube Studies of the Reactions of $H_3O^+$, $NO^+$ and $O_2^+$ with a Series of Volatile Carboxylic Acids and Esters," *Int. J. Mass Spectrom. Ion Process.* 172, 137-147 (1998).

$H_3O^+ + M$
$NO^+, O_2^+ + M$
9 Carboxylic Acids
8 Esters
Rate Constants
Product Ions

(78836) Penning Ionization, Cross Sections, Band Assignments, Energy Dependences

$He(2^3S) + C_{10}H_8$
$He(2^3S) + C_{14}H_{10}$

78616. Aguillon, F., "A New Treatment of Nonadiabatic Dynamics: Application to the Determination of the $He^+ + H_2 \rightarrow He + H + H^+$ Differential Cross Section," *J. Chem. Phys.* 109, 560-571 (1998).

$He^+ + H_2(v \leq 4)$
Reaction Dynamics
$H + H^+$ Products
Cross Sections
Calculations

(78848) *f*-Values, 124, 280 nm Doublets, Calculations

$Mg^+(3p^2P\text{-}3s^2S)$
$Mg^+(4p^2P\text{-}3s^2S)$

78617. Chu, Y., G. Senn, P. Scheier, A. Stamatovic, T.D. Mark, "Dissociative Electron Attachment to NO Molecules and NO Clusters," *Phys. Rev. A: At. Mol. Opt. Phys.* 57, R697-700 (1998).

$NO + e^-$
$(NO)_n + e^-$
Dissociative Attachment
$O^- + N(^2D)$
Products

78618. Continetti, R.E., "Photoelectron-Photofragment Coincidence Studies of Dissociation Dynamics," *Int. Rev. Phys. Chem.* 17, 227-260 (1998).

$NO^-.N_2O, N_3O_2^-$
$O_3^-, O_4^-$
Dissociation Dynamics
Photodetachment
Transient Species Studies
Review

78619. Krishnamurthy, M., V.M. Bierbaum and S.R. Leone, "Vibrational State Dependence of the $N_2^+(v=0\text{-}3) + HCl$ Reaction at Thermal Energies," *Chem. Phys. Lett.* 281, 49-56 (1997).

$N_2^+(v=0\text{-}3) + HCl$
Reactive Relaxation
Rate Constants
Branching Ratios

(79197) Vibrational Relaxation, v=0-4, Charge Transfer Rate Constants, Multiquantum Channels

$N_2^+(v) + N_2, O_2$

78620. Bruning, F., S. Matejcik, E. Illenberger, Y. Chu, G. Senn, D. Muigg, G. Denifl and T.D. Mark, "Effects of Temperature on the Dissociative Electron Attachment to $N_2O$," *Chem. Phys. Lett.* 292, 177-182 (1998).

$N_2O + e^-$
Dissociative Attachment
T Dependence
Mechanisms

(79098) Hollow Cathode, Major Species, Measurements, Kinetic Model

$N_2O$ Discharge

78621. Magnier, S., M. Persico and N. Rahman, "Quantum Wavepacket Dynamics Simulations of Above-Threshold Dissociation in $Na_2^+$," *Chem. Phys. Lett.* 279, 361-366 (1997).

$Na_2^+$
Above Threshold Dissociation
Channels
$(1^2\Sigma_g^+ \rightarrow 1^2\Sigma_u^+ \rightarrow 1^2\Pi_g)$
2-Photon Process
Na(3p) Product

(78758) Ionization, Crossed Beams, Electron Transfer, n≤100

$Na_n + C_{60}, C_{84}$
$Na_n + TCNQ, Br_2, SF_6$

78622. Tarnovsky, V., H. Deutsch and K. Becker, "Electron Impact Ionization of the Hydroxyl Radical," *J. Chem. Phys.* 109, 932-936 (1998).

$OD + e^-$
$D_2O + e^-$
Ionization
Cross Sections

78623. Guberman, S.L., "Mechanism for the Green Glow of the Upper Ionosphere," *Science* 278, 1276-1278 (1997).

$O_2^+ + e^-$
Rate Constant
$O(^1S)$ Product
Yield

78624. Miller, T.M., J.V. Seeley, W.B. Knighton, R.F. Meads, A.A. Viggiano, R.A. Morris, J.M. Van Doren, J. Gu and H.F. Schaefer III, "Electron Attachment to $PCl_3$ and $POCl_3$, 296-552 K," *J. Chem. Phys.* 109, 578-584 (1998).

$PCl_3 + e^-$
$POCl_3 + e^-$
Dissociative Attachment
Rate Constants
Measurements
$PCl_n, POCl_n$
$PCl_n^-, POCl_n^-$
Structural Calculations
EAS

78625. Morris, R.A., and A.A. Viggiano, "Chemistry of $PO^-$, $PO_2^-$ and $PO_3^-$ in the Gas Phase," *J. Chem. Phys.* 109, 4126-4127 (1998).

$PO^-, PO_2^- + M$
$PO_3^- + M$
M = Numerous Neutrals
Rate Constants

78626. Fairley, D.A., G.B.I. Scott, D.B. Milligan, R.G.A.R. Maclagan and M.J. McEwan, "Selected Ion Flow Drift Tube Study of the $SO_2^+/H_2$ H-Atom Abstraction Reaction," *Int. J. Mass Spectrom. Ion Process.* 172, 79-87 (1998).

$SO_2^+ + H_2$
Rate Constant
Energy Barrier
P.E. Surface

(78843) Lifetimes, Oscillator Strengths

$Si^+(3s^24s^2S_{1/2})$
$Si^+(3s^25s^2S_{1/2})$

78627. Tsuji, M., M. Ide, E. Oda and Y. Nishimura, "Formation of XeBr*, Xe* and Br* by the $Xe^+(^2P_{1/2})/Br^-$/He and $Xe^+(^2P_{3/2})/Br^-$/He Three-Body Ionic-Recombination Reactions in a Helium Flowing Afterglow," *J. Chem. Phys.* 109, 3374-3385 (1998).

$Xe^+(^2P_{1/2}) + Cl^- + He$
$Xe^+(^2P_{3/2}) + Cl^- + He$
Product XeBr(B,D)
$Xe(^3P_1, ^1D_2), Br(^2P_{1/2})$
Branching Ratios
Mechanisms

## 16. INHIBITION/ADDITIVES

(See also Section 21 for Combustion Emission Control Additives)

| | | |
|---|---|---|
| (78499) | Polymer Combustion, Ignition, Emissions, Review | Retardants |
| (79090) | $CH_3OH$, $C_2H_5OH/O_2$, Additive Perturbations | NO Effects |
| 78628. | Babushok, V., W. Tsang, G.T. Linteris and D. Reinelt, "Chemical Limits to Flame Inhibition," *Combust. Flame* 115, 551-560 (1998). | Flame Inhibition<br>Chemical Cycles<br>$CH_4$/Air<br>Relative Efficiencies<br>Optimal Rates |
| 78629. | Takahashi, K., T. Inomata, T. Abe, H. Fukaya, E. Hayashi and T. Ono, "Inhibition of Combustion by Bromine-Free Polyfluorocarbons. II. Burning Velocities of Methane and *n*-Heptane Flames with Polyfluorocarbons Containing Oxygen, Nitrogen or Sulfur," *Combust. Sci. Technol.* 131, 187-191 (1998). | Inhibition<br>$CH_4$,*n*-$C_7H_{16}$ Flames<br>$(CF_3)_3N$,$(CF_3)_2NCF_2H$<br>$(C_2F_5)_2O$,$CF_3SF_5$<br>$C_2F_5SF_5$ Effects<br>Burning Velocities |
| (78669) | $CH_4/O_2$ Atmospheric Oxidation Rates, Halide Enhancements | Cl,Br |
| (78909) | $CH_4/CHCl_3/O_2/N_2$ Flames, Temperatures, Species Profiles, Probe Sampling, Kinetic Modeling, Data/Model Comparisons | $CHCl_3$ Effects |
| 78630. | Rumminger, M.D., D. Reinelt, V. Babushok and G.T. Linteris, "Numerical Study of the Inhibition of Premixed and Diffusion Flames by Iron Pentacarbonyl," *Combust. Flame* 116, 207-219 (1999). | Inhibition<br>$CH_4/O_2/N_2$<br>$Fe(CO)_5$<br>Mechanism<br>Kinetic Model |
| (78549) | $CH_4$/Air Counterflow Flame, Modeling | Water Droplet Extinction |
| 78631. | MacDonald, M.A., T.M. Jayaweera, E.M. Fisher and F.C. Gouldin, "Inhibition of Nonpremixed Flames by Phosphorus-Containing Compounds," *Combust. Flame* 116, 166-176 (1999). | Inhibition<br>$CH_4$/Air<br>$(CH_3O)_3PO$<br>$(CH_3O)_2P(O)CH_3$<br>Extinction<br>Strain Rates |
| (78584) | Detonations, CO, $H_2/O_2$/Ar, Velocities | Halocarbon Effects |
| (78465) | Coal Pyrolysis, HCN, $NH_3$,$N_2$ Emission Releases | NaOH,KOH,$Ca(OH)_2$ Seeding Effects |
| (78918) | Petroleum Coke, Slow Pyrolysis, Oxidation, HCN, $NH_3$, NO, $N_2O$ Formation | $CaCO_3$ Effects |
| (78523) | Ignition Delays, $H_2$/High Temperature Supersonic Air | $CO_2$,$H_2$,$H_2O_2$ Additive Effects |

(78901) $H_2/N_2O$/Ar Flames, NO, NH, OH, O, Major Species Profiles, Measurements, Modeling — $NH_3$ Effects

(79036) Isomerization, Catalyzed by CO or $CO_2$ Additions, Collision Energy Effects — $HCN^+/HNC^+$

(78672) Atmospheric Crystallization, Promoted by $(NH_4)_2SO_4$ but not Soot — $NH_4NO_3$

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Deposition
Oil Fired
Boiler Fouling
Deposit Analysis

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Carbon Deposition
Coke Ovens
Particle/Coal Gas
Increased
Adhesion
Effects

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Flame Spread
Liquid Fuels
Thermocapillary
Fluid Forces
Modeling

(78568) Turbulent Buoyancy Driven Flames, Scaling Laws — Ceiling Fire

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Liquid Fuel
Surface
Vaporization
$CH_3OH$,*n*-$C_5H_{12}$
Convective
Diffusion

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Fire Spread
Wood Fuels
Controlling
Parameters
Wind Tunnel

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Insulation
Lagging Material
Fuel Spread
Ignition
Modeling

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Flame Spread
PMMA
Leading Flame Edge
Fuel Movement Effects

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Impinging Jet/ Wall Flames
Reynolds Number Effects
Modeling

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Surface Monitoring
Adsorbed $I_2$
Cavity Ringdown Method
Sensitivity

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Heterogeneous
$BrNO_2/NaNO_3$,KBr(s)
$BrNO_2/KNO_2$,KCl(s)
$ClNO_2/KNO_2$,KBr(s)
$ClNO_2$/KCl(s)
Uptake Coefficients
Products

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Heterogeneous
$C_2H_2$ ,$C_2H_4/Al_2O_3$(s)
$C_2H_2/O_3/Al_2O_3$(s)
$C_2H_4/O_3/Al_2O_3$(s)
Reaction Probabilities

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Heterogeneous
$ClONO_2$/Aerosols
Fast Flow Reactor
Uptake Method
Data Analysis Treatment

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$ClONO_2$/Ice
$HNO_3$ ,$N_2O_5$/Ice
$HNO_3/H_2O$ Product
Uptake Coefficients

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| (78670) | HCl(g) Product, Measurements, Atmospheric Role | $HNO_3$(g)/NaCl(s) |
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| 78649. | ten Brink, H.M., "Reactive Uptake of $HNO_3$ and $H_2SO_4$ in Sea-Salt (NaCl) Particles," *J. Aerosol Sci.* 29, 57-64 (1998). | Heterogeneous<br>$HNO_3$/NaCl(s)<br>$H_2SO_4$/NaCl(s)<br>Uptake<br>Coefficients<br>Reactions |
| (78682) | Atmospheric Heterogeneous Sources of $Cl_2$, $Br_2$ and BrCl | $O_3$/NaBr(s) + hν<br>$O_3$/NaCl(s) + hν |
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(See also Section 10 for Ignition)

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I.C. Engine
$H_2$ Fueled
Constant Power
Low Emissions
Assessments

78659. Chan, S.H., and X.S. Chen, "Prediction of Mixture Formation and Heat Release in a Turbocharged Direct Injection Diesel Engine," *J. Inst. Energy* 71, 33-46 (1998).

Diesel Engine
DI Turbocharged
Combustion
Model

78660. Buzukov, A.A., and B.P. Timoshenko, "Effect of Secondary Mixing on Fuel Ignition and Combustion in a Diesel Engine," *Combust. Expl. Shock Waves, Russia* 33, 26-33 (1997).

Diesel Engine
Curved Wall/
Incident Jet
Improved Mixing
Ignition

78661. Naber, J.D., and D.L. Siebers, "Hydrogen Combustion under Diesel Engine Conditions," *Int. J. Hydrogen Energy* 23, 363-371 (1998).

Diesel Engine
$H_2$ Fueled
Auto-ignition
Delay Times
Emissions

78662. Kittelson, D.B., "Engines and Nanoparticles: A Review," *J. Aerosol Sci.* 29, 575-588 (1998).

Diesel Engines
Particle Emissions
Nanosizes
Potential Regulation
Review

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Diesel Engines
Soot Trap
Two Stage
Oxidation
Regeneration Method

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Diesel Engines
Soot Traps
$H_2O_2$ Regeneration
Kinetic Rates

## 20. PLUME/STACK CHEMISTRY/ATMOSPHERIC EMISSIONS

(78726) Fossil/Biomass Combustion, Soot Formation, Atmosphere/Ocean Records

Ocean Sediment
Cycle

(78874) Laser Ablation, ICP/Mass Analyzer, Atomic Analysis Method

Atmospheric
Particles

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Stratospheric
$CCl_4$,$CH_4$,H-1211
CFC-11,-12,-113
$CH_3CCl_3$,$N_2O$,$SF_6$
Lifetimes
Measurements

| | | |
|---|---|---|
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| (78956) | 2-Methyl-3-buten-2-ol, Atmospheric Lifetime, Rate Constants for Reactions with OH, $O_3$, $NO_3$ and Cl | $(CH_3)_2C(OH)CHCH_2$ |
| (78971) | Atmospheric Lifetimes, $(CH_2COOCH_3)_2$, $CH_2(CH_2COOCH_3)_2$, $(CH_2CH_2COOCH_3)_2$, Rate Constants for Reactions with OH | Dibasic Esters |
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| 78671. | Nikolaev, Yu.A., and P.A. Fomin, "The Nature of Noctilucent Clouds and the Earth's Ozone Layer," *Combust. Expl. Shock Waves, Russia* 33, 393-402 (1997). | Upper Atmospheric $H_2$ Combustion $H_2O,O_3$ Source Term |
| (78799) | Infrared Spectra, Atmospheric Implications, Calculations | $H_2O.O_2$ $H_2O.N_2$ |

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Atmospheric
$NH_4NO_3$
Crystallization
$(NH_4)_2SO_4$ Promotion
Negligible Soot Effects

78673. Vnukov, A.K., and F.A. Rozanova, "Calculation of Ground Level $NO_x$ Concentrations from Low Level Sources," *Thermal Eng., Russia* 44, 984-986 (1997).

Smoke Plumes
$NO/NO_2$
Conversion
$O_3$ Oxidation

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Stratospheric
$NO/NO_y$ Ratios
Aircraft Emission Enhancements
Measurements
Modeling

(78860) Chemiluminescent Detector, Gold Converter Method

$NO,NO_y$
Aircraft Emissions

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Atmospheric
$N_2O$
Anthropogenic
$NO_x$ Source Role
Estimations

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Atmospheric
$N_2O,NO_y,O_3$
Chemical Coupling
Time Scales

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Upper Troposphere
$OH,HO_2$
Sources
$H_2O_2,CH_3OOH$
Role
NO Effects
$O_3$ Enhancements

78678. Roelofs, G.-J., J. Lelieveld and R. van Dorland, "A Three-Dimensional Chemistry/General Circulation Model Simulation of Anthropogenically Derived Ozone in the Troposphere and Its Radiative Climate Forcing," *J. Geophys. Res.* 102, 23389-23401 (1997).

Tropospheric
$O_3$
Anthropogenic
Source Strengths
Climate Role

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Stratospheric
$O_3$
Depletions
Greenhouse
Warming
Interplay

78680. Fish, D.J., and M.R. Burton, "The Effect of Uncertainties in Kinetic and Photochemical Data on Model Predictions of Stratospheric Ozone Depletion," *J. Geophys. Res.* 102, 25537-25542 (1997).

Stratospheric
$O_3$
3-D Modeling
Depletion
Uncertainties

78681. Barrie, L., and U. Platt, "Arctic Tropospheric Chemistry: An Overview," *Tellus B. Chem. Phys. Meteor.* 49, 450-454 (1997).

Tropospheric
$O_3$
Arctic Depletion
Chemistry
Review

78682. Oum, K.W., M.J. Lakin, D.O. DeHaan, T. Brauers and B.J. Finlayson-Pitts, "Formation of Molecular Chlorine from the Photolysis of Ozone and Aqueous Seat Salt Particles," *Science* 279, 74-77 (1998).

Atmospheric
$O_3 + NaBr(s) + h\nu$
$O_3 + NaCl(s) + h\nu$
Heterogeneous
Sources
$Cl_2, Br_2, BrCl$

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Renewable
Energy Sources
$CO_2$ Reduction
Policy Impacts
Economics

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Climatic Impact
600 Year History
Variability

78685. Bird, M.I., and J.A. Cali, "A Million Year Record of Fire in Sub-Saharan Africa," *Nature* 394, 767-769 (1998).

Climatic Impact
$CO_2$
Million Year
Biomass
Nature Fires
Analysis

78686. Hansen, J.E., M. Sato, R. Ruedy, A. Lacis and J. Glascoe, "Global Climate Data and Models: A Reconciliation," *Science* 281, 930-932 (1998).

Climatic Impact
Global Warming
Satellite/
Ground Base
Data Reconciliation

78687. Hansen, J., M. Sato, R. Ruedy, A. Lacis, K. Asamoah, K. Beckford, S. Borenstein, E. Brown, B. Cairns, B. Carlson, B. Curran, S. de Castro, L. Druyan, P. Etwarrow, T. Ferede, M. Fox, D. Gaffen, J. Glascoe, H. Gordon, S. Hollandsworth, X. Jiang, C. Johnson, N. Lawrence, J. Lean, J. Lerner, K. Lo, J. Logan, A. Luckett, M.P. McCormick, R. McPeters, R. Miller, P. Minnis, I. Ramberran, G. Russell, P. Russell, P. Stone, I. Tegen, S. Thomas, L. Thomason, A. Thompson, J. Wilder, R. Willson and J. Zawodny, "Forcings and Chaos in Interannual to Decadal Climate Change," *J. Geophys. Res.* 102, 25679-25720 (1997).

Climatic Change
Forcings,Chaos
Roles
Model
Predictions

78688. Schimel, D.S., "The Carbon Equation," *Nature* 393, 208-209 (1998).

Climatic Impact
Carbon Cycle
Ocean/Land
Role,Questions

78689. Sarmiento, J.L., T.M.C. Hughes, R.J. Stouffer and S. Manabe, "Simulated Response of the Ocean Carbon Cycle to Anthropogenic Climate Warming," *Nature* 393, 245-249 (1998).

Climatic Impact
$CO_2$
Ocean Role
Warming Effects

78690. Cao, M., and F.I. Woodward, "Dynamic Responses of Terrestrial Ecosystem Carbon Cycling to Global Climate Change," *Nature* 393, 249-252 (1998).

Climatic Impact
$CO_2$
Ecosystem
Feedback
Changes

78691. Steinberg, M., "Technologies for Reducing Carbon Dioxide Emissions from Fossil Fuel Fired Installations," in *Hydrogen Energy System: Production and Utilization of Hydrogen and Future Aspects*, Y. Yurum, ed., Proceedings of a Conference Held in Akcay, Turkey, August 1994, 21 Papers, 341 pp., *NATO Adv. Study Instit. Ser. E. Appl. Sci.* 295, 53-68 (1995).

Climatic Impact
$CO_2$
Mitigation
Technologies
Biomass/Fossil
Fuel Conversions
$CH_3OH + C(s)$
Products

78692. Berntsen, T.K., I.S.A. Isaksen, G. Myhre, J.S. Fuglestvedt, F. Stordal, T.A. Larsen, R.S. Freckleton and K.P. Shine, "Effects of Anthropogenic Emissions on Tropospheric Ozone and Its Radiative Forcing," *J. Geophys. Res.* 102, 28101-28126 (1997).

Climatic Impact
Tropospheric
$O_3$
Historical Changes
Radiative Forcing
Effects

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Climatic Impact
Tropospheric
$O_3$ ,$SO_4^{2-}$ Aerosols
Radiative Forcing
Modeling

## 21. COMBUSTION EMISSIONS/$NO_X$, $SO_2$ CHEMISTRY, CONTROL

(See also Section 3 for Burner Emissions and Section 19 for Engine Emissions)

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| 78695. | Kawaguchi, O., T. Ohtani and H. Kojima, "Thermal Decomposition Process of a Polyethylene Pellet in a Hot Stagnation Flow," *Combust. Sci. Technol.* 130, 411-421 (1997). | Incineration<br>Polyethylene<br>Pyrolysis<br>Melting<br>Dissociation |
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| (78685) | Million Year Record of Natural Fires, $CO_2$ Climatic Impact Analysis | Biomass |
| 78698. | Olsson, J.G., U. Jaglid, J.B.C. Pettersson and P. Hald, "Alkali Metal Emission during Pyrolysis of Biomass," *Energy Fuels* 11, 779-784 (1997). | Alkali Metal<br>Release<br>Biomass<br>Pyrolysis<br>Cl Enhancement<br>Effects |
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| (78737) | Soot, Polyaromatics Formation | Biomass Combustion |
| (78912) | $C_3H_8$/$O_2$/Ar Flames, Kinetic Modeling, Data Comparisons | PAH,Aromatics<br>Emissions |

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PAH Formation
$C_{10}H_8$/Plasma Arc Discharges
Fullerenes
Soot Analysis

(78899) $CH_4$/Air/$C_6H_5R$ Flames, R=H, $CH_3$, $C_2H_5$, $C_2H_3$, $C_2H$, Hydrocarbon Profiles, Soot Fractions, Mechanisms

$C_{10}H_8$,Soot Emissions

78701. Bjorkman, E., and B. Stromberg, "Release of Chlorine from Biomass at Pyrolysis and Gasification Conditions," *Energy Fuels* 11, 1026-1032 (1997).

Chlorine
Release
Biomass
Pyrolysis
Gasification

78702. Christensen, K.A., M. Stenholm and H. Livbjerg, "The Formation of Submicron Aerosol Particles, HCl and $SO_2$ in Straw-Fired Boilers," *J. Aerosol Sci.* 29, 421-444 (1998).

HCl,$SO_2$
$K_2SO_4$/KCl Particle Emissions
Straw Combustion

78703. McQuay, M.Q., R.K. Dubey and W.A. Nazeer, "An Experimental Study on the Impact of Acoustics and Spray Quality on the Emissions of CO and NO from an Ethanol Spray Flame," *Fuel* 77, 425-435 (1998).

CO,NO Emissions
$C_2H_5OH$ Spray Flame
Rijke Tube
Nozzle/Acoustic Effects

(78465) Coal Pyrolysis, NaOH, KOH, $Ca(OH)_2$ Seeding Effects

HCN,$NH_3$,$N_2$ Emission Releases

(78918) Petroleum Coke, Slow Pyrolysis, Oxidation, $CaCO_3$ Effects

HCN,$NH_3$,NO,$N_2O$ Formation

78704. Bradley, D., P.H. Gaskell, X.J. Gu, M. Lawes and M.J. Scott, "Premixed Turbulent Flame Instability and NO Formation in a Lean-Burn Swirl Burner," *Combust. Flame* 115, 515-538 (1998).

NO Formation
Rotating Matrix Burner
Turbulent Swirl Flow
Measurements
Model

(78579) Stabilization of Turbulent Lean Flames, Fuel Injection Strategies

NO Formation

78705. Kuligowski, F.F., and N.M. Laurendeau, "Effect of Oxygen Content on $NO_x$ Emission Index for Nonpremixed $CH_4$/$O_2$/$N_2$ Flames," *Combust. Sci. Technol.* 130, 423-430 (1997).

$NO_x$ Formation
$CH_4$/$O_2$/$N_2$
$O_2$ Content Effects

(78907) $CH_4$/Air, Thermal, Prompt, Kinetic Modeling, Reduced Scheme

$NO_x$ Formation

(78908) $CH_4$/Air, Kinetic Modeling, Mechanism

NO Formation

| | | |
|---|---|---|
| (78900) | $C_2H_6/O_2/N_2$ Inverse Diffusion Flames, Temperature Profiles, Saturated LIF Measurements | NO Formation |
| (78527) | Strained $C_3H_8$/Air Interface, Ignition Modes, Structure, Asymptotic Analysis | $NO/NO_2$ Formation |
| 78706. | Munts, V.A., Yu.G. Lekomtseva and A.P. Baskakov, "Formation of Nitrogen Oxides in Burning Solid Fuel," *Thermal Eng., Russia* 44, 993-998 (1997). | NO Formation<br>Coal,Shales<br>FBC<br>Generalized Correlations |
| (78906) | Pulverized Coal Flames, $HCN/NH_3$ Conversion, Kinetic Modeling, Reduced Scheme | NO Formation |
| 78707. | Courtemanche, B., and Y.A. Levendis, "A Laboratory Study on the NO, $NO_2$, $SO_2$, CO and $CO_2$ Emissions from the Combustion of Pulverized Coal, Municipal Waste Plastics and Tires," *Fuel* 77, 183-196 (1998). | $NO,NO_2,SO_2$<br>$CO,CO_2$<br>Emissions<br>Pulverized Coal<br>Tire,Plastics<br>Combustion<br>Measurements |
| 78708. | Mallet, C., M. Aho, J. Hamalainen, J.P. Rouan and J.-R. Richard, "Formation of NO, $NO_2$ and $N_2O$ from Gardanne Lignite and Its Char under Pressurized Conditions," *Energy Fuels* 11, 792-800 (1997). | $NO,NO_2,N_2O$<br>Formation<br>Lignite,Char<br>Thermobalance<br>Measurements<br>Parameter Dependences |
| 78709. | Pedersen, L.S., D.J. Morgan, W.L. van de Kamp, J. Christensen, P. Jesperson and K. Dam-Johansen, "Effects on $SO_x$ and $NO_x$ Emissions by Co-Firing Straw and Pulverized Coal," *Energy Fuels* 11, 439-446 (1997). | $NO_x,SO_x$<br>Formation<br>Straw/Coal<br>Co-firing Effects |
| 78710. | Takami, H., T. Suzuki, Y. Itaya and M. Hasatani, "Performance of Flammability of Kerosene and $NO_x$ Emission in the Porous Burner," *Fuel* 77, 165-171 (1998). | $NO_x$ Formation<br>Porous Ceramic Burner<br>Kerosene Fuel<br>Equilibrium<br>Behavior |
| (78901) | Major Species, $H_2/N_2O$/Ar Flame Profiles, $NH_3$ Additive Effects, Measurements, Modeling | NO,NH,OH,O |
| (78674) | $NO/NO_y$ Stratospheric Enhancements, Measurements, Modeling | Aircraft Emissions |
| 78711. | Ziemann, J., F. Shum, M. Moore, D. Kluyskens, D. Thomaier, N. Zarzalis and H. Eberius, "Low $NO_x$ Combustors for Hydrogen Fueled Aero Engine," *Int. J. Hydrogen Energy* 23, 281-288 (1998). | Low $NO_x$<br>Emissions<br>Aero Engines<br>$H_2$ Fuel |

78712. Dahl, G., and F. Suttrop, "Engine Control and Low $NO_x$ Combustion for Hydrogen Fueled Aircraft Gas Turbines," *Int. J. Hydrogen Energy* 23, 695-704 (1998).

Low $NO_x$
Aircraft Emissions
$H_2$ Fuel
Developments

78713. St. John, D., and S. Samuelsen, "Robust Optimal Control of a Natural Gas-Fired Burner for the Control of Oxides of Nitrogen ($NO_x$)," *Combust. Sci. Technol.* 128, 1-21 (1997).

$NO_x$ Control
Swirl Stabilized
Natural Gas
Swirl/Excess Air
Optimization
Algorithm

78714. Keer, A., R. Bautista, L.Y. Manzanares, E.S. Garbett and J. Swithenbank, "$NO_x$ Reduction in a Pulverized Coal Swirl Burner with High Velocity Jets," *J. Inst. Energy* 71, 71-80 (1998).

$NO_x$ Control
Pulverized Coal
Swirl Burner
Flowfield Velocities

78715. Seo, A., and K. Hase, "Study on $NO_x$ Reduction in Reburning," *Combust. Sci. Technol.* 131, 381-393 (1998).

$NO_x$ Control
Reburn Method
Kinetics
Measurements

78716. Weber, R., G. Wecel, A. Verlaan, F. Breussin and J. Dugue, "Experimental and Numerical Studies on Reburn Jet Penetration and Mixing with Application to Boilers and Municipal Waste Incinerators," *J. Inst. Energy* 71, 94-109 (1998).

$NO_x$ Control
Reburn Method
Jet Mixing
Flowfield
CFD Adequacy

78717. Alzueta, M.U., H. Rojel, P.G. Kristensen, P. Glarborg and K. Dam-Johansen, "Laboratory Study of the $CO/NH_3/NO/O_2$ System: Implications for Hybrid Reburn/SNCR Strategies," *Energy Fuels* 11, 716-723 (1997).

$NO_x$ Control
Reburn/$NH_3$
Hybrid
Performance
Measurements

78718. Ehrhardt, K., M. Toqan, P. Jansohn, J.D. Teare, J.M. Beer, G. Sybon and W. Leuckel, "Modeling of $NO_x$ Reburning in a Pilot Scale Furnace Using Detailed Reaction Kinetics," *Combust. Sci. Technol.* 131, 131-146 (1998).

NO Control
Injected Reburn
$CH_4/NH_3$ Method
Turbulent
$CH_4$ Diffusion
Kinetic Modeling

78719. Bilbao, R., A. Millera, M.U. Alzueta and L. Prada, "Evaluation of the Use of Different Hydrocarbon Fuels for Gas Reburning," *Fuel* 76, 1401-1407 (1997).

$NO_x$ Control
Reburn Method
$CH_4, C_2H_6$
$C_2H_4, C_2H_2$
Effectiveness
T Effects

78720. Glarborg, P., M.U. Alzueta, K. Dam-Johansen and J.A. Miller, "Kinetic Modeling of Hydrocarbon/Nitric Oxide Interactions in a Flow Reactor," *Combust. Flame* 115, 1-27 (1998).

NO Control
Reburn Conditions
NO/Hydrocarbon
Dominant Channels
Kinetic Modeling

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NO Control
$NO/H_2, CH_4, CO/Ar$
Heated Flow Reactor
Metal 3-Way Catalyst
$NO/N_2O, HCN, NH_3$ Conversions
$O_2$ Effects

78722. Misono, M., H. Niiro and Y. Hirao, "Mechanism of Reduction of Nitrogen Oxides with Propene in Excess Oxygen Catalyzed by Bifunctional Catalysts," *Research Chem. Intermed* 24, 123-132 (1998).

$NO_x$ Control
$C_3H_6$/Zeolite
Development
Mechanisms

78723. Luo, J., S.L. Suib, M. Marquez, Y. Hayashi and H. Matsumoto, "Decomposition of $NO_x$ with Low Temperature Plasmas at Atmospheric Pressure: Neat and in the Presence of Oxidants, Reductants, Water and Carbon Dioxide," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7954-7963 (1998).

$NO_x$ Control
Discharge Method
$C, CO_2, C_2H_6$
$H_2O, O_2$
Effects
Kinetics

78724. Lyngfelt, A., L.-E. Amand and B. Leckner, "Reversed Air Staging: A Method for Reduction of $N_2O$ Emissions from Fluidized Bed Combustion of Coal," *Fuel* 77, 953-959 (1998).

$N_2O$ Control
FBC
Coal Fueled
Reversed Air Staging
Efficiencies

## 22. SOOT, DIAMOND, PARTICLE FORMATION/CONTROL

(See also Section 19 for Soot Formation in Engines)

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Soot Formation
Flames
Aerosol
Gelation
Aggregation Rates

78726. Masiello, C.A., and E.R.M. Druffel, "Black Carbon in Deep-Sea Sediments," *Science* 280, 1911-1913 (1998).

Soot
Fossil/Biomass
Combustion
Atmospheric
Ocean Sediment
Cycle

78727. Brookes, S.J., and J.B. Moss, "Measurements of Soot Production and Thermal Radiation from Confined Turbulent Jet Diffusion Flames of Methane," *Combust. Flame* 116, 49-61 (1999).

Soot Formation
Turbulent Jet
$CH_4$/Air
Thermal Radiation
Measurements

| | | |
|---|---|---|
| 78728. | Kaplan, C.R., G. Patnaik and K. Kailasanath, "Universal Relationships in Sooting Methane/Air Diffusion Flames," *Combust. Sci. Technol.* 131, 39-65 (1998). | Soot Formation<br>$CH_4$/Air<br>Diffusion Flame<br>Structure<br>Species Profiles<br>Flamelet Model |
| 78729. | Xu, F., K.-C. Lin and G.M. Faeth, "Soot Formation in Laminar Premixed Methane/Oxygen Flames at Atmospheric Pressure," *Combust. Flame* 115, 195-209 (1998). | Soot Formation<br>$CH_4/O_2$<br>Volume Fractions<br>Major Species<br>Profiles<br>Measurements |
| 78730. | Nemeth, A., and K. Heberger, "Computer Modeling of Formation of Soot Precursors in the Oxidation of Methane," *Ber. Bunsenges. Phys. Chem.* 102, 257-261 (1998). | Soot Formation<br>Precursors<br>$CH_4/O_2$<br>Kinetic Modeling<br>Aromatic Radicals<br>Automatic<br>Reaction Mechanism<br>Generator |
| 78731. | Hepp, H., and K. Siegmann, "Mapping of Soot Particles in a Weakly Sooting Diffusion Flame by Aerosol Techniques," *Combust. Flame* 115, 275-283 (1998). | Soot Formation<br>$CH_4$/Ar/Air<br>Diffusion Flame<br>Size<br>Distributions |
| (78898) | $CH_4$ Diffusion Flame, Opposed Flow, Species Profiles, PAHS, Aromatics | Soot Fractions |
| (78530) | Volume Fractions, $CH_4$ /$C_4$ Hydrocarbons/Air Diffusion Flames, Temperatures, Stable Species, $C_2H_2/C_6H_6$ Equilibrium Mechanisms | Soot Formation |
| 78732. | McEnally, C.S., and L.D. Pfefferle, "An Experimental Study in Nonpremixed Flames of Hydrocarbon Growth Processes that Involve Five-Membered Carbon Rings," *Combust. Sci. Technol.* 131, 323-344 (1998). | Soot,PAH<br>Formation<br>$CH_4$/M/Air<br>M = *c*-$C_5H_{10}$, *c*-$C_5H_8$, *c*-$C_5H_7CH_3$, *c*-$C_9H_8$<br>$C_5$ Ring Effects<br>Measurements |
| (78899) | $CH_4$/Air/$C_6H_5R$ Flames, R = H, $CH_3$, $C_2H_5$, $C_2H_3$, $C_2H$, Hydrocarbon Profiles, $C_{10}H_8$ Formation, Mechanisms | Soot Fractions |
| (78611) | Low Pressure $C_2H_2/O_2$ Premixed Flames, Beam Sampling, Mass Analysis | PAH Cations |
| 78733. | Mitrovic, A., and T.-W. Lee, "Soot Formation Characteristics of Laminar Partially Premixed Flames," *Combust. Flame* 115, 437-442 (1998). | Soot Formation<br>$C_2H_4$/Air<br>Jet Flows<br>Volume Fractions<br>Mapping |

78734. De Iuliis, S., M. Barbini, S. Benecchi, F. Cignoli and G. Zizak, "Determination of the Soot Volume Fraction in an Ethylene Diffusion Flame by Multiwavelength Analysis of Soot Radiation," *Combust. Flame* 115, 253-261 (1998).

Soot Formation
$C_2H_4$
Diffusion Flame
Volume Fractions
Multiwavelength
Emission Method

78735. Dobbins, R.A., R.A. Fletcher and H.-C. Chang, "The Evolution of Soot Precursor Particles in a Diffusion Flame," *Combust. Flame* 115, 285-298 (1998).

Soot Formation
$C_2H_4$
Diffusion Flame
Precursor
Intermediates
Probe Sampling
Mass Analysis

78736. Krestinin, A.V., P.A. Tesner and S.V. Shurupov, "Formation of Carbon Black in Ethylene and Diacetylene Pyrolysis," *Kinet. Catal., Russia* 39, 1-3 (1998).

Soot Formation
$C_2H_4$ ,$C_4H_2$
Pyrolysis
Yields

78737. Kozinski, J.A., and R. Saade, "Effect of Biomass Burning on the Formation of Soot Particles and Heavy Hydrocarbons: An Experimental Study," *Fuel* 77, 225-237 (1998).

Soot Formation
Polyaromatics
Biomass
Combustion

(78755) Graphite Arc/He,Ar, Kinetic Model

Fullerene
Formation

(78700) $C_{10}H_8$ Plasma Arc Discharges, PAH, Fullerene Products

Soot Formation

78738. Vander Wal, R.L., T.M. Ticich and A.B. Stephens, "Can Soot Primary Particle Size be Determined by Laser Induced Incandescence?," *Combust. Flame* 116, 291-296 (1999).

Soot Formation
Sizes
LII/TEM
Measurement
Comparisons
Diffusion Flames

78739. Saito, M., M. Sato and A. Nishimura, "Soot Suppression by Acoustic Oscillated Combustion," *Fuel* 77, 973-978 (1998).

Soot
Suppression
$C_2H_2$ Flames
Acoustic
Oscillation
Effects

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Diamond Formation
Nonequilibrium
Thermodynamic
Model
Phase Diagrams

78741. Che, S., O. Sakurai, K. Shinozaki and N. Mizutani, "Particle Structure Control Through Intraparticle Reactions by Spray Pyrolysis," *J. Aerosol Sci.* 29, 271-278 (1998).

Particle Formation
Spray Pyrolysis
Evaporative/
Sintering Control
Particle Morphology

78742. Glumac, N.G., Y.-J. Chen, G. Skandan and B. Kear, "Scalable High-Rate Production of Non-Agglomerated Nanopowders in Low Pressure Flames," *Mater. Lett.* 34, 148-153 (1998).

$Al_2O_3$,$SiO_2$
$TiO_2$
Nanopowders
Low Pressure
Flame Formation

78743. Kennedy, I.M., Y. Zhang, A.D. Jones, D.P.Y. Chang, P.B. Kelly and Y. Yoon, "Morphology of Chromium Emissions from a Laminar Hydrogen Diffusion Flame," *Combust. Flame* 116, 233-242 (1999).

$Cr_2O_3$
Flame Particle
Formation
Morphology
Cenospheres
Sizes

78744. Alexandrescu, R., I. Morjan, A. Crunteanu, S. Cojocaru, S. Petcu, V. Teodorescu, F. Huisken, B. Kohn, M. Ehbrecht, "Iron Oxide Based Nanoparticles Produced by Pulsed Infrared Laser Pyrolysis of $Fe(CO)_5$," *Mater. Chem. Phys.* 55, 115-121 (1998).

$Fe_2O_3$
Particle Formation
IR MPD
$Fe(CO)_5/SF_6$
Sizes

78745. Helble, J.J., "Combustion Aerosol Synthesis of Nanoscale Ceramic Powders," *J. Aerosol Sci.* 29, 721-736 (1998).

$MgO$,$TiO_2$,$ZrO_2$
Ceramic Powders
Nanoscale
Flame Synthesis
Particle Sizes
Review

78746. Spicer, P.T., C. Artelt, S. Sanders and S.E. Pratsinis, "Flame Synthesis of Composite Carbon Black-Fumed Silica Nanostructured Particles," *J. Aerosol Sci.* 29, 647-659 (1998).

$SiO_2/C$
Nanosize
Composite
Particles
$C_2H_2/O_2/SiCl_4$
Synthesis
Review

## 23. PARTICLE CHARACTERIZATION

(See also Section 5 for Spray Characterization)

78747. Burtscher, H., S. Kunzel and C. Huglin, "Characterization of Particles in Combustion Engine Exhaust," *J. Aerosol Sci.* 29, 389-396 (1998).

Engine
Particle
Emissions
Analysis Methods

(78662) Diesel Engine Emissions, Potential Regulation, Review

Nanosize Particles

(78872) Particulate Evaporation Rates, ICP/AES Slurry Nebulizer, Modeling Code Calibration — $Al_2O_3$, SiC

78748. Rotundi, A., F.J.M. Rietmeijer, L. Colangeli, V. Mennella, P. Palumbo and E. Bussoletti, "Identification of Carbon Forms in Soot Materials of Astrophysical Interest," *Astron. Astrophys.* 329, 1087-1096 (1998). — Soot; Carbon Structures; Analysis

78749. D'Alessio, A., A. D'Anna, G. Gambi and P. Minutolo, "The Spectroscopic Characterization of Ultraviolet Absorbing Nanoparticles in Fuel Rich Soot Forming Flames," *J. Aerosol Sci.* 29, 397-409 (1998). — Nanoparticles; Rich Sooting Flames; UV Spectral Characteristics; Presoot Region Sizes

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(78672) Atmospheric Crystallization, Promoted by $(NH_4)_2SO_4$ but not Soot — $NH_4NO_3$

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## 24. NUCLEATION/COAGULATION/CLUSTERS

(See also Section 22 for Nucleation and Growth of Particles, Section 26 for Spectroscopy of Cluster Molecules and Section 44 for Cluster Structures)

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(79024) Unimolecular Dissociation, Blackbody Radiative Initiation Evidence — Ion Clusters

78753. Viggiano, A.A., S.T. Arnold and R.A. Morris, "Reactions of Mass-Selected Cluster Ions in a Thermal Bath Gas," *Int. Rev. Phys. Chem.* 17, 147-184 (1998). — Cluster Anions; $(H_2O)_n^-$; $CO_3^-(H_2O)_n$; $X^-(H_2O)_n$; Detachment; Thermal Dissociation; Rate Constants; Channels; Review

| | | |
|---|---|---|
| (78833) | Predissociation Rates, CN(A) Product, Lifetimes | $CN(B).Ar_n$ |
| (79028) | $O+C_2H_4$ Half Reaction, $CH_2CHO$ Vinoxyl Product Radical LIF, ps Pump/Probe Method | $C_2H_4.NO_2+h\nu$ |
| (79004) | IR MPA/MPI, Autoionization Rates, Electronically Excited State Roles | $C_{60}$ |
| (79191) | Vibrational Relaxation, Efficiencies, Calculations | $C_{70}(v)+He,Ar$ |
| 78754. | Krestinin, A.V., and A.P. Moravsky, "Mechanism of Fullerene Synthesis in the Arc Reactor," *Chem. Phys. Lett.* 286, 479-484 (1998). | Fullerenes<br>Synthesis<br>Carbon Arc<br>Model |
| 78755. | Sukhinin, G.I., and O.A. Nerushev, "A Model for the Formation of Fullerenes in Carbon Vapor," *J. Appl. Mech. Techn. Phys., Russia* 38, 625-637 (1997). | Fullerene<br>Formation<br>Graphite Arc/<br>He,Ar<br>Kinetic Model |
| (78700) | $C_{10}H_8$ Plasma Arc Discharges, PAH Formation, Soot Analysis | Fullerenes |
| (78610) | Photoionization, $e^-$ Ionization, Ion Fragmentation Efficiencies, Review | Fullerenes,PAHS |
| (79118) | P.E. Curves, Ion Pair State Effects | $Cl_2.He;Cl_2.Ne$<br>$Cl_2.Ar$ |
| (79194) | Lifetime, Vibrational Relaxation Cross Sections for $H_2(v)+He$, Low Temperatures | $H_2(v).He$ |
| (79070) | Photodetachment Transition State Probing of Reaction Dynamics | $H_3O^-$<br>$OH^-(H_2)$ |
| (79231) | Dissociation Energies, 3-Electron Bonds, DFT Failures | $He_2^+,Ne_2^+,Ar_2^+$<br>$(H_2O)_2^+,(HCl)_2^+,(HF)_2^+$<br>$(H_2S)_2^+,(NH_3)_2^+,(PH_3)_2^+$ |
| (78994) | Photoinitiation Absorption Spectrum, LiF Product, Mechanism | $Li.HF+h\nu$ |
| 78756. | Shin, D.N., R.L. DeLeon and J.F. Garvey, "Observation of Magic Numbers within $NO/NH_3$ Mixed Cluster Ions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7772-7778 (1998). | $NO^+(NH_3)_n$<br>Magic Numbers<br>n=3-28<br>$NH_3$ Loss<br>Rate Constants |
| 78757. | Angel, L., and A.J. Stace, "The Critical Hydration Reactions of $NO^+$ and $NO_2^+$," *J. Chem. Phys.* 109, 1713-1715 (1998). | $NO^+(H_2O)_{3-5}$<br>$NO_2^+(H_2O)_{2-4}$<br>Collision Induced<br>Fragmentation<br>$HNO_2,HNO_3$<br>Formation<br>Critical Cluster<br>Size |

(78618) Photodetachment, Dissociation Dynamics, Transient Species Studies, Review
$NO^-.N_2O$
$O_3^-, O_4^-$

(78617) Dissociative Attachment, $O^- + N(^2D)$ Products
$(NO)_n + e^-$
$NO + e^-$

78758. Hampe, O., P. Gerhardt, S. Gilb and M.M. Kappes, "Ion-Pair Formation in Near-Thermal Energy Collisions of Sodium Clusters with Electron Acceptors," *J. Chem. Phys.* 109, 3485-3496 (1998).
$Na_n + C_{60}, C_{84}$
$Na_n + TCNQ, Br_2, SF_6$
Crossed Beam
Ionization
Electron Transfer
$n \leq 100$

(79082) Reaction Dynamics, Reactivities, Activation Energies
$Pd_3, Pt_3 + CH_4$
$Pd_3, Pt_3 + H_2$

(78841) (78842) Lifetimes, Predissociation, Cluster Effects, Measurements
SH.Rg(A)
SD.Rg(A)

## 25. FLAME/CHEMILUMINESCENT SPECTROSCOPY

(79022) Chemiluminescence, Sr + NOCl, Vibrational Distributions, Branching Ratio, Rotational Alignment
SrCl(B,A-X)

## 26. SPECTRAL CHARACTERIZATIONS/ANALYSES

(See also Section 43 for Energy Levels and Theoretically Calculated Spectral Constants, and Section 44 for Vibrational Frequencies and Constants)

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Rydberg States
Long Lived
Stabilization
ZEKE Method

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Jahn-Teller
Vibronic
Interactions
$CH_3O, C_6H_6^+$
$P_4^+$
Overview

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$Eu, NO, O_2$

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Polarizabilities
$BCl, CCl^+$
$CP^-, PO^+$
Dipole Moments
Calculations

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$C_2H_4$ ,$C_6H_6$
$C_{10}H_8$
Geometries
Calculations

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Polarizabilities
Alkanes
Group Additivity
Estimation
Method

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ArKr
Photoelectron Spectra
6 Vibrational Progressions
State Assignments
Spectral Constants
IPS

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$AsH_3$
FTIR Spectrum
Assignments

(78829) ODR Spectrum, Radiative Lifetime

$BaCl(G^2\Sigma^+)$

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CFBr(A-X)
LIF Spectra
Constants
Jet Cooled
Lifetimes
P.E. Surface
$\Delta H_f$(CFBr)

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$CF_2$(A-X)
LIF Spectrum
Frequency
Assignments

(78938) Infrared Absorption Coefficient

$CF_3$

(78890) CARS and Optoacoustic Raman Spectra, Frequencies, Monitors

$CHF_2Cl$
$CH_3CF_2Cl$

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$CH_2$(b-a)
Diode Laser
Modulated
Absorption
Assignments
Constants

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$CH_2Br_2$,$CH_2I_2$
$CH_2BrI$
Absorption
Cross Sections
Atmospheric
Lifetimes

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$CH_3$,$\nu_2$
Absorption
Pulsed Pyrolysis
Nozzle Expansion
Modulation
Method

(79215) PFI-PE Spectra, IPS

$CH_3SH$,$C_2H_5SH$

(79216) Negative Ion Photoelectron Spectra, EAS, Energies, $\Delta H_f$(HCN,$CN_2$)

$CN_2$,$CHN_2$

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CO(e,d,a′a)
Emission Spectra
Assignments
Spectral Constants
Matrix Study

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$CO_2$/He,Ar
$\Sigma$-$\Sigma$ IR Bands
Line Mixing Effects
Collisional Model

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V System
Vibrational
Analysis
Revised
Assignments

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$CD_3CDO(S_1\text{-}S_0)$
Vibronic Bands
Analysis
$CH_3CHO(S_1)$
v,J Lifetimes

(79002) Visible Luminescence, Assignment, IR MPD $C_2H_2Cl_2F_2$

$CF_2ClCH$

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$C_2H_2(X)$
Bending Dynamics
Polyads
Analysis

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$C_2H_2(v)$

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$C_2H_2Cl_2$
IR Spectra
4 Isotopomers
Constants
Structure

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*c*-$C_2H_2N_4$, *c*-$C_4H_4N_2$
$C_6H_6$, $C_6H_5NH_2$
Organics
Electronic
Spectroscopy
Laser/Jet Cooling
Methods

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$CH_2CHO$
5 $CH_3$-Substituted
Vinoxy Radicals
LIF Spectra
O + Alkene
Radical
Observation

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$CH_3CO_2I^-$
Absorption
Cross Sections
Photoproducts

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*c*-$C_2H_4O$
Rotational
Spectrum
Constants

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$(CH_3)_2O$
Rotational
Spectrum
Constants
Partition Functions

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$C_3$(A-X)
LIF Spectrum
Jet Cooled
Assignments
A-State Constants

(78954) Infrared Spectrum, Calculations

$CH_3COCH_2O_2NO_2$

(78884) Absorption, Cavity Ringdown, 2-D Array Spectra

$C_3H_8$(6ν),635 nm

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*t*-$C_4H_9COCH_3$
IR,Raman
Spectra
Vibrational
Assignments

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$C_{10}H$,$C_{10}D$($^2\Pi$-X)
Cavity Ringdown
Absorption Spectra
Band Origins

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Jahn-Teller
Vibronic
Coupling
Theory

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Electronic
Absorption
Spectra
200-800 nm
Calculations

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$X^2\Sigma^+$ Spectral Constants
$D_0$
Calculations

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$CaOC_2H_5$(C-X)
CaCCH(C-X)
Laser Spectroscopy
Frequencies
S/O Splitting
Constants

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CdHe(B,A-X)
Laser Excitation
Spectra
Constants
$D_e'$,$D_e''$

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Continuum Emission
$e^-$ Beam Excitation

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ClF(E,f-Y,B,C)
Bound-Free
Emission
OODR Spectra
E($v' \leq 8$),f($v' \leq 5$)
P.E. Curves

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$ClO_2$(A-X)
LIF Spectrum
Constants
Matrix Study

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CrCl($X^6\Sigma^+$)
Rotational
Spectrum
Constants
$^{35}Cl$,$^{37}Cl$ Values

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CrNO,CrON
NCrO
Product Isomers
FTIR Spectra
Laser Ablation
Matrix Study

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OODR Spectra
Constants
P.E. Curves
$(C/1_u)$ Perturbations

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$FH_2^-$
Photoelectron
Spectrum
P.E. Surface
Simulations
Accuracies

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$HN_3$,$DN_3$
VUV Absorption
Spectra
NH,ND(c,A)
Quantum Yields
Mechanisms

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$H_2NS$,$D_2NS$
Rotational
Spectra
Constants
Geometries

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$H_2O.O_2$
$H_2O.N_2$
IR Spectra
Calculations
Atmospheric
Implications

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KCCH
KCCD
Rotational
Spectrum
Constants

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KS
Rotational
Spectrum
Constants

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$K_2(C\text{-}1^1\Pi_g)$
LIF Spectra
$1^1\Pi_g$ Constants
RKR P.E. Curve
$v'' \leq 107$
$D_e, T_e(1^1\Pi_g)$

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LiMg
Resonant
Photoionization
Spectral Constants
(F,E-X) Bands
$D_0$"

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MoO
WO(B,A′,A,X)
Absorption
Spectral Constants

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$NH_3^+, ND_3^+$
Vibronic Structure
Photoelectron
Spectra
Frequency
Assignments
Constants

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NO(B-X)
Absorption
Cross Sections
160-195 nm
Term Values
Spectral Constants
Oscillator
Strengths

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NO(T,$Z^2\Sigma^+$)
Rydberg States
Term Values
ASE Decay
(T-R),(Z-Y)
Nearby States

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NO
Rydberg States
2-Color RFWM
Energy Levels
Decay Rates
Absorption
Cross Sections

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NO
Rydberg States
Long Lived
ZEKE States
Control Method

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$N_2$
Raman Spectra
High Pressure
Measurements

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$N_2^+$(A-X)
Velocity
Modulation
Spectral Constants
$T_{Trans,Vib,Rot}$

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$N_2H^+$
Rotational
Spectrum
Pulsed Slit
Supersonic Expansion
Modulation
Method

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$NaCH_3$
$NaCD_3$
Rotational
Absorption Spectra
Constants
Geometries

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$Na_2(5^1\Pi_u, 6^1\Sigma_u^+)$
$Na_2(7^1\Sigma_u^+)$
Triple Resonance
Spectra
Level Assignments
Constants

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Rotational
Spectra
Dunham Constants
Isotopes

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$OH(v=2)+H_2$
Entrance Channel
Collision Complex
IR Spectrum
Lifetime

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$O_2$
Absorption
Cross Sections
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T Dependences

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$O_2^+(c,v=0,1)$
PFI-PE Spectrum
Linewidths
Spectral Constants
Predissociation
Lifetimes
IPS

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$O_2^+(X)$-$O_2(a)$
Photoelectron
Spectra
Rydberg State
Autoionization

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$O_3(^3A_2$-X)
Absorption
Lineshapes
Predissociative
Lifetime

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$(O_2)_2$
630,578 nm
Intracavity
Absorption Spectra
$D_0'$,$D_0''$

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$SF_2$
(2+1)REMPI
8 Electronic
Band Systems
Assignments
IP

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$SO_2(^1B_1$-X)
SV LIF Spectra
100 Levels
30400-34230 $cm^{-1}$
Jet Cooling
Assignments

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$SbH_3$
Rotational Spectrum
Constants
Geometry

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$Sr^+Ar_n$,n=2-8
Photofragment
Cross Sections
Measurements
Theory
Structures

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$VAr^+$(B-X)
Spectral Analysis
Constants
$D_0'$,$D_0''$

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$Xe_2$
Rydberg States
REMPI/TOF
PES Spectra
Assignments
Constants

## 27. EXCITED STATE LIFETIMES/QUENCHING

(See also Section 45 for Vibrational and Rotational Relaxation Processes)

(79040) Reaction Dynamics, Conical Intersections, Probabilities, Testing of Four Methods

$M^* + H_2 / M + H_2(v,J)$
$M^* + H_2 / MH + H$

(79114) Low-lying States, Transition Probabilities, Lifetimes, Calculations

AlSi

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$Ar(^3P_{2,0}) + MCN$
M=Na,K,Rb
CN(B,v) Product
Mechanism

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BaCl(G)
Radiative
Lifetime
ODR Spectrum

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$Br_2$,$Cl_2$(B-X)
IBr,ICl(B-X)
Magnetic Field
Quenching Effects
Lifetimes

(78766) Lifetimes, (A-X) LIF Spectra, Constants, Jet Cooled, P.E. Surface, $\Delta H_f$ (CFBr)

CFBr(A),v

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CH(B)
v=0,J≤21;v=1,J≤13
2-Color RFWM
Predissociative
Lifetimes

(79042) Reaction Dynamics, Rate Constants, Intermediates, Lifetimes

$^1CH_2 + C_2H_2$

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$CH_2(a) + H_2S, NH_3$
$CH_2(a) + M$
$M = RNO_2, RSH, RCN$
$(CH_3)_2S, (CH_3)_2S_2$
12 Reactions
Rate Constants

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$CN(B).Ar_n$
Predissociation
Rates
CN(A) Product
Lifetimes

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$CO^+(X,v)$
Radiative
Lifetime
Measurements

(79172) E-E Transfer, Triplet State Formation, Phosphorescence

$C_2H_2(A/a)$

(79173) E-E Transfer, fs 200 nm Pump, Ultrafast Decay Channels

$C_2H_4^*, C_2H_3Cl^*$

(78774) Lifetimes, LIF, Supersonic Jet

$CH_3CHO(S_1),v,J$

(79112) Quenching Cross Sections, P.E. Curve Calculations

$Cl(^2P_{1/2}) + Rg$

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$Dy, Dy^+$
Radiative
Lifetimes
440 Levels
LIF Measurements

(79058) Reaction Dynamics, Scattering Hyperquantization Algorithm

$F(^2P_{1/2,3/2}) + H_2$

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$He(2^3S) + C_{10}H_8$
$He(2^3S) + C_{14}H_{10}$
Penning Ionization
Cross Sections
Band Assignments
Energy Dependences

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$N(^2D,^2P)+C_2H_2$
$N(^2D,^2P)+C_2D_2$
Rate Constants
T Dependences

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$NCl(a)+F,Cl$
$NCl(a)+NCl(a)$
Quenching
$Cl+N_3$
Rate Constants
NCl(a) Product Branching Ratio

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$NCl(a)+I$
$Cl+N_3$
Rate Constants
T Dependence
$I(^2P_{1/2})$ Yields

(79174) E-E Transfer, Gateway States, Magnetic Field Effects

NO(B/a)

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$O(^1D)+CH_4$
Crossed Beams
H-Atom Elimination
$CH_2OH/CH_3O$ Channels

(78853) $v'=13,14,N$, Predissociation Linewidths, (B-X), 3 Comparative Studies

$O_2(B)$

(79080) Transition States, P.E. Surfaces, Energies, Reaction Dynamics

$^1O_2+R_2S$

(78818) Predissociative Lifetimes, PFI-PE Spectrum, Linewidths, Constants, IPS

$O_2^+(c,v=0,1)$

(78820) Predissociative Lifetime, $(^3A_2$-X) Absorption Lineshapes

$O_3(^3A_2)$

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SH.Rg(A)
SD.Rg(A)
Lifetimes
Cluster Effects
Measurements

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SH.Rg(A)
SD.Rg(A)
Lifetimes
Predissociation
Blocking
Calculations

(79175) E-E Transfer, v,J Relaxation, $SO_2$(A) Lifetimes, Rate Constants

$SO_2$(A/a)

78843. Schectman, R.M., H.S. Povolny and L.J. Curtis, "Selected Lifetime and Oscillator Strength Measurements in $Si^+$," *Astrophys. J.* 504, 921-924 (1998).
$Si^+(3s^24s^2S_{1/2})$
$Si^+(3s^25s^2S_{1/2})$
Lifetimes
Oscillator Strengths

(78627) XeBr(B,D), $Xe(^3P_1,^1D_2)$, $Br(^2P_{1/2})$ Product Branching Ratios, Mechanisms
$Xe^+(^2P_{1/2})+Cl^-+He$
$Xe^+(^2P_{3/2})+Cl^-+He$

(79176) E-E Transfer, Intersystem Crossing, Matrix Study
$Zn(^1P_1/^3P_J)/Rg$

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(See also Section 27 for Lifetimes and Transition Probabilities)

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$Co^+$
11 Transitions
Oscillator Strengths
Measurements

78845. Biemont, E., D.C. Morton and P. Quinet, "Ultraviolet Transitions of Astrophysical Interest in $Ge^+$, $As^+$ and $Se^+$," *Mon. Not. Roy. Astron. Soc.* 297, 713-731 (1998).
$Ge^+$,$As^+$,$Se^+$
Oscillator Strengths
Transitions
Calculations

(79121) $^{1,3}$ Transition Probabilities, P.E. Surfaces
$HOCl(^3A',^3A'',X^1A')$

78846. Astashkevich, S.A., N.V. Kokina and B.P. Lavrov, "Semiempirical Determination of Absolute Values of the Dipole Moments of the ($3d^1\Pi_g \rightarrow 2p^1\Sigma_u^+$, $3d^1\Pi_g \rightarrow 2p^1\Pi_u$, and $3d^1\Delta_g \rightarrow 2p^1\Pi_u$) Electronic Transitions in the Hydrogen Molecule," *Opt. Spectrosc., Russia* 83, 837-843 (1997).
$H_2(^1\Pi_g\text{-}^1\Sigma_u^+,^1\Pi_u)$
$H_2(^1\Delta_g\text{-}^1\Pi_u)$
Transition Dipole Moments
Analysis

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$Li_2(^3\Sigma\text{-}X^1\Sigma)$
Oscillator Strengths
$Li_2(v,J)$
Kinetically Cold
Photoassociation
Spontaneous Decay
Formation Method

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$Mg^+(4p^2P\text{-}3s^2S)$
124,280 nm Doublets
*f*-Values
Calculations

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NO($np^2\Pi^+$-A)
Oscillator Strengths
Measurement Method

(78806) Oscillator Strengths, 160-195 nm Absorption Cross Sections, Spectral Constants

NO(B-X)

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NO(X,v≤20)
$\Delta v = 1\text{-}4$
Einstein A-Coefficients
Dipole Moment Function
Data Fitting

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OH(A-X)
OD(A-X)
v,J Transition Probabilities
Transition Moment Measurements
Theory

(79129) Low-lying Quarter States, P.E. Curves, Spectral Constants, F.C. Factors, A-Coefficients

$^4SO^+$

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$S_2O$(C-X)
F.C. Factors
LIF Spectra
Method

## 29. LINESHAPES/STRENGTHS

(79135) IR Intensities, Frequencies, Structural Calculations, Geometry, $D_e$

$Al_2O_4$

(79137) IR Intensities, Frequencies, Geometry, $\Delta H_f$, Structural Calculations

$BrONO_2$

(79144) Infrared Intensities, Geometries, Energies, Structural Calculations

CCOH(A,X)

(79151) CHO, $CH_2OH$, OH, O Group Substitution Effects, Frequencies, IR Intensities, Structural Calculations

$C_{10}H_8$, $C_{10}H_8^+$

(79152) N, CN, NH, $NH_2$ Group Substitution Effects, IR Frequencies, Relative Intensities, Structural Calculations

$C_{10}H_8$, $C_{14}H_{10}$

(79153) IR Intensities, Neutrals/Cations, Isomers, Frequencies, H-Atom Loss Effects, Structural Calculations

$C_{10}H_7CH_3$
$C_{14}H_9CH_3$

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$O_2$(B-X)
v′=13,14,N
Predissociation
Linewidths
3 Comparative
Studies

(78818) PFI-PE Spectrum, Linewidths, Predissociation Lifetimes, Constants, IPS

$O_2^+$(c,v=0,1)

(78820) Absorption Lineshapes, Predissociative Lifetimes

$O_3(^3A_2\text{-}X)$

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Rb($^2P_{3/2,1/2}$-$^2S_{1/2}$)
Broadening
Coefficients
He,$N_2$,Xe
Colliders
Measurements

## 30. ANALYSIS/MONITORING TECHNIQUES

(See also Section 32 for Mapping and Tomographic Methods)

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H Atom
Flame Monitor
$Sr^+/SrOH^+$
Ion Method
Burning Velocity/
H Correlation

(78747) Engine Emissions, Analysis Methods

Particles

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Electrospray
Negative Ion
Analysis Method
$F^-$,$Cl^-$,$Br^-$,$I^-$
$ClO_3^-$,$ClO_4^-$,$IO_3^-$
Linearity
Detection Limits

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Gas Chromatography
Flame Sampling
Mass Analysis
Comparisons
Assessments

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$C_2H_2$(v)
Combination Bands
Vibrational
Enhancement
Monitoring
Method

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REMPI
$BrO, Br_2$
Monitor

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Chemiluminescent Detector
$NO, NO_y$
Aircraft Measurements
Gold Converter Method

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Chemiluminescence
$O_3$
Analysis
Gas/Solution
Methods,Review

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Laser Induced Breakdown Spectra
Atomic Analysis
Advances
Review

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Laser Induced Breakdown Spectra
Analysis Method
Metals
Applications
Review

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Laser Induced Breakdown Spectra
Atomic Analysis
Advances
Review

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Laser Induced Breakdown Spectra
Analysis Method
Solid/Liquid/Gas
Detection Limits

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Atomic Emission
Analysis
Review
434 References

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Atomic Emission
Analysis
Glow Discharge
Sensitivities

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Atomic Emission
RF Glow Discharge
N,O,S
Monitor
Solid Samples
Method

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Atomic Emission
Analysis
He Discharges
Excitation/
Rotational
Temperatures
Ag,Pb
Detection Limits

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ICP
Thermochemical
Calculations
70 Elements
Ionization
Extents

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ICP/AES
Sample Preparation
Interferences
Review

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ICP/AES
Slurry Nebulizer
$Al_2O_3$,SiC
Particulate
Evaporation
Modeling Code
Calibration

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ICP/
Mass Analysis
Ar/Air Plasma
Ion Source

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ICP/
Mass Analysis
Atmospheric
Particles
Laser Ablation
Atomic Analysis

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Atomic Absorption
Fluorescence
Analysis
Review
703 References

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Absorption
Diode Lasers
24 Molecules
Detection Limits
Modulation Schemes

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Thermogravimetry/ FTIR
Analysis Method
History
Review

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FTIR
Analysis Method
Multicomponent
Organic
Gaseous Mixtures

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FTIR Absorption
$CF_3CHBrCl$
$CHF_2OCHClCF_3$
$N_2O$
Monitoring

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Atomic Absorption
$C_2H_2/N_2O$
Analysis Flame
Historical
Development
Review

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Self Absorption
Doppler Shift
$He(2^3S)$
Glow Discharge
Monitor
Comparisons

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Absorption
Cavity Ringdown
ICP
Source
Utilization

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Absorption
Optothermal
Polarization
LIF,REMPI
Cavity Ringdown
$C_2HD,C_2H_2,CO_2$
Heterodyne
Monitoring Methods

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Absorption
Cavity Ringdown
2-D Array Spectra
$C_3H_8$(6v),635 nm

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$H^-$
Cavity Ringdown
Laser Absorption
Photodetachment
Density Monitor

(78640) Absorption, Surface $I_2$ Monitoring, Sensitivity

Cavity Ringdown

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Atomic Analysis
LIF,LIBS
LEI
Overview

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2-Photon LIF
BrO(C-X)
Monitor
$O(^1D) + CF_3Br$
$Br + O_3$
Sources

(78979) 2-Photon 205.1 nm Method, $C_2H_3$, $C_3H_5$, HCOOH, $H_2S$, Simultaneous Photolysis and H Monitor, H Product Energies

H-Atom LIF

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Fluorescence
Hg
Monitor
Hg Source Lamp
Sensitivity

(78900) Saturated LIF, $C_2H_6/O_2/N_2$ Inverse Diffusion Flames, Temperature Profiles

NO

(78577) Time Resolved, Turbulent $CH_4$/Air Flame

ps LIF,OH

78889. Sharafutdinov, R.G., A.A. Ilyukhin, V.V. Smirnov, A.E. Belikov, G.I. Sukhinin and R.L. Pykhov, "Populations of Rotational Levels of Nitrogen Molecules in Free Jets: Comparison of CARS and Electron Beam Fluorescent Technique," *Chem. Phys.* 233, 127-144 (1998).

CARS,Raman
$e^-$-Beam,LIF
$N_2$(J)
Populations
Comparisons
Free Jet Beams

78890. Melchior, A., I. Bar and S. Rosenwaks, "$CHF_2Cl$ and $CH_3CF_2Cl$ Detection by Coherent Anti-Stokes Raman Scattering and Photoacoustic Raman Spectroscopy, " *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7273-7276 (1998).

CARS
Optoacoustic Raman
$CHF_2Cl$
$CH_3CF_2Cl$
Frequencies
Monitors

78891. Schmitt, M., G. Knopp, A. Materny and W. Kiefer, "Femtosecond Time-Resolved Four-Wave Mixing Spectroscopy in Iodine Vapor," *Chem. Phys. Lett.* 280, 339-347 (1997).

fs DFWM
$I_2$
(B,X) Wavepacket Dynamics
Monitoring Method

78892. Fernee, M.J., P.F. Barker, A.E.W. Knight and H. Rubinsztein-Dunlop, "Sensitive Detection of Sodium in a Flame Using Parametric Four-Wave Mixing and Seeded Parametric Four-Wave Mixing," *Phys. Rev. A: At. Mol. Opt. Phys.* 57, 2802-2813 (1998).

DFWM
Na
Flame Monitor
Comparison
2 Methods
Sensitivities

## 31. FLAME CONCENTRATION MEASUREMENTS

(See also Section 34 for Flame Species Profiles)

78893. Turbiez, A., J.F. Pauwels, L.R. Sochet, S. Poitou and M. Perrin, "Chemical Structure of Laminar Premixed Natural Gas Flames: Influence of Equivalence Ratio," *Bull. Soc. Chim. Belg.* 106, 355-360 (1997).

Species Profiles
Natural Gas
Premixed Flames
3 Stoichiometries
Beam Sampling
Kinetic Model Comparisons

78894. L'Esperance, D., B.A. Williams and J.W. Fleming, "Detection of Fluorocarbon Intermediates in Low Pressure Premixed Flames by Laser Induced Fluorescence," *Chem. Phys. Lett.* 280, 113-118 (1997).

Species Profiles
CF,CHF,$CF_2$,$COF_2$
$CH_4/O_2/M$
$M = CH_{4-n}F_n, n = 1\text{-}3$
LIF Monitor

78895. Bhargava, A., and P.R. Westmoreland, "Molecular Beam Mass Spectrometer Analysis of a Fuel-Lean Ethylene Flame," *Combust. Flame* 115, 456-467 (1998).

Species Profiles
$C_2H_4/O_2/Ar$
Molecular Beam Mass Analysis
$C_2H_4 + H,OH$
$C_2H_3 \rightarrow$
Rate Constants

78896. Lin, K.-C., and G.M. Faeth, "Structure of Laminar Premanently Blue, Opposed-Jet Ethylene Fueled Diffusion Flames," *Combust. Flame* 115, 468-480 (1998).

Species Profiles
$C_2H_4$/Air
Opposed Jet
Soot Free
Gas Velocities
Measurements
Kinetic Model Comparisons

78897. Walravens, B., J. Vandooren and P.J. Van Tiggelen, "Peculiar Features in Lean Butane Flames," *Combust. Sci. Technol.* 130, 399-409 (1997).

Species Profiles
*n*-,*iso*-$C_4H_{10}/O_2$
Low Pressure Flames
$(CH_3)_2CO$,$C_4H_8$
Intermediates
Kinetics

78898. Vincitore, A.M., and S.M. Senkan, "Experimental Studies of the Micro-Structures of Opposed Flow Diffusion Flames: Methane," *Combust. Sci. Technol.* 130, 233-246 (1997).

PAHS,Aromatics
Soot Fractions
Species Profiles
Opposed Flow
$CH_4$ Diffusion Flame

78899. McEnally, C.S., and L.D. Pfefferle, "Experimental Assessment of Naphthalene Formation Mechanisms in Nonpremixed Flames," *Combust. Sci. Technol.* 128, 257-278 (1997).

$C_{10}H_8$ Formation
$CH_4/Air/C_6H_5R$
$R = H, CH_3, C_2H_5, C_2H_3, C_2H$
HC Flame Profiles
Soot Fractions
Mechanisms

78900. Partridge Jr, W.P., J.R. Reisel and N.M. Laurendeau, "Laser Saturated Fluorescence Measurements of Nitric Oxide in an Inverse Diffusion Flame," *Combust. Flame* 116, 282-290 (1999).

NO,Temperature Profiles
$C_2H_6/O_2/N_2$
Inverse Diffusion
Saturated
LIF

78901. Venizelos, D.T., and R.C. Sausa, "Laser Induced Fluorescence, Mass Spectrometric and Modeling Studies of Neat and $NH_3$-Doped $H_2/N_2O$/Ar Flames," *Combust. Flame* 115, 313-326 (1998).

NO,NH,OH,O
Major Species
Flame Profiles
$H_2/N_2O$/Ar
$NH_3$ Effects
Measurements
Modeling

## 32. MAPPING/TOMOGRAPHIC METHODS

78902. Torniainen, E.D., and F.C. Gouldin, "Tomographic Reconstruction of 2-D Absorption Coefficient Distributions from a Limited Set of Infrared Absorption Data," *Combust. Sci. Technol.* 131, 85-105 (1998).

Tomography
IR Absorption
Inversion Method
$CH_4$/Ar Flows
Accuracies

78903. Tse, S.D., R.A. Anthenien, A.C. Fernandez-Pello and K. Miyasaka, "An Application of Ultrasonic Tomographic Imaging to Study Smoldering Combustion," *Combust. Flame* 116, 120-135 (1999).

Tomographic
Imaging
Propagation
Smoldering
Combustion
Polyurethane
Foam

| | | |
|---|---|---|
| (78535) | Cellular Structures, Video Images, Circular Porous Plug Burner | Flame Imaging |
| (79010) | Fragment Ion Imaging Method, $Cl_2+h\nu$, Product Angular Alignment, State Symmetries | Cl |
| (79011) | Ion Imaging Method, Product Energy, Angular Distributions, $Cl_2O+h\nu$, $HOCl+h\nu$ | $Cl(^2P_{1/2,3/2})$ |
| (78580) | Turbulent $H_2$/Ar Jet Diffusion Flames, Reynolds Number Effects | PLIF,OH |
| (78534) | Triple Flames, PIV Velocities, Measurements, Modeling | PLIF,OH |

## 33. OPTOGALVANIC/OPTOACOUSTIC METHODS

## 34. FLAME KINETIC MODELING

| | | |
|---|---|---|
| 78904. | Yousefian, V., "A Rate-Controlled Constrained-Equilibrium Thermochemistry Algorithm for Complex Reacting Systems," *Combust. Flame* 115, 66-80 (1998). | Kinetic Modeling<br>Partially Equilibrated<br>Reduced Mechanism<br>Algorithm<br>CO Kinetic Quenching<br>Accuracies |
| 78905. | Yossefi, D., M.R. Belmont, S.J. Maskell and G. Ben-Dor, "Stimulation and Implementation of Laminar Flow Reactors for the Study of Combustion Systems of Ethane, Methane and Deborane," *Fuel* 77, 173-181 (1998). | Kinetic Modeling<br>$B_2H_6$/Air<br>$CH_4$,$C_2H_6$/$O_2$/$CO_2$<br>$C_2H_6$/Air<br>Flow Reactor<br>Transport Code<br>Performance |
| 78906. | Pedersen, L.S., P. Glarborg and K. Dam-Johansen, "A Reduced Reaction Scheme for Volatile Nitrogen Conversion in Coal Combustion," *Combust. Sci. Technol.* 131, 193-223 (1998). | Kinetic Modeling<br>NO Formation<br>Pulverized Coal Flames<br>HCN/$NH_3$<br>Conversion<br>Reduced Scheme |
| 78907. | Romero, C.E., "Reduced Kinetic Mechanism for $NO_x$ Formation in Laminar Premixed $CH_4$/Air Flames," *Fuel* 77, 669-675 (1998). | Kinetic Modeling<br>$CH_4$/Air<br>$NO_x$ Formation<br>Thermal,Prompt<br>Reduced Scheme |
| 78908. | Levin, V.A., G.D. Smekhov and A.N. Khmelevskii, "Simulation of Nitric Oxide Formation in Combustion of Methane/Air Mixtures," *Combust. Expl. Shock Waves, Russia* 33, 9-18 (1997). | Kinetic Modeling<br>$CH_4$/Air<br>NO Formation<br>Mechanism |

| | | |
|---|---|---|
| 78909. | Devynck, P., J.F. Pauwels and L.R. Sochet, "Chemical Structure of a Stoichiometric Low Pressure $CH_4/CHCl_3/O_2/N_2$ Flame," *Bull. Soc. Chim. Belg.* 106, 361-366 (1997). | Kinetic Modeling<br>$CH_4/CHCl_3/O_2/N_2$<br>T,Species Profiles<br>Probe Sampling<br>Data/Model Comparisons |
| (78720) | Kinetic Modeling, Hydrocarbon Injected Reburn Process, Dominant NO/Hydrocarbon Channels, NO Control | $CH_4, C_2H_6/O_2$ |
| (78718) | Kinetic Modeling, $CH_4/NH_3$ Injected Reburn Process, Turbulent Diffusion Flame, NO Control | $CH_4$/Air |
| 78910. | Reisel, J.R., C.D. Carter and N.M. Laurendeau, "Measurements and Modeling of OH and NO in Premixed $C_2H_6/O_2/N_2$ Flames at Atmospheric Pressure," *Energy Fuels* 11, 1092-1100 (1997). | Kinetic Modeling<br>$C_2H_6/O_2/N_2$<br>LIF,OH,NO<br>T Profiles<br>Data Fitting Adequacies |
| 78911. | Barbe, P., F. Baronnet, R. Martin and D. Perrin, "Kinetics and Modeling of the Thermal Reaction of Propene at 800 K. III. Propene in the Presence of Small Amounts of Oxygen," *Int. J. Chem. Kinet.* 30, 503-522 (1998). | Kinetic Modeling<br>$C_3H_6/O_2$<br>Product Formation<br>Mechanism<br>Measurements<br>Rate Constants |
| 78912. | Marinov, N.M., M.J. Castaldi, C.F. Melius and W. Tsang, "Aromatic and Polycyclic Aromatic Hydrocarbon Formation in a Premixed Propane Flame," *Combust. Sci. Technol.* 128, 295-342 (1997). | Kinetic Modeling<br>$C_3H_8/O_2/Ar$<br>PAH,Aromatics<br>Formation<br>Data Comparisons |
| 78913. | Zils, R., R. Martin and D. Perrin, "Kinetic Study and Modeling of the Hetero-Homogeneous Pyrolysis and Oxidation of Isobutane around 800 K. I. Pyrolysis in an Unpacked Pyrex Reactor," *Int. J. Chem. Kinet.* 30, 425-437 (1998). | Kinetic Modeling<br>*i*-$C_4H_{10}$<br>Pyrolysis<br>Self-Inhibition<br>Data Fitting |
| 78914. | Dagaut, P., M. McGuinness, J.M. Simmie and M. Cathonnet, "The Ignition and Oxidation of Tetrahydropyran: Experiments and Kinetic Modeling," *Combust. Sci. Technol.* 129, 1-16 (1997). | Kinetic Modeling<br>*c*-$C_5H_{10}O/O_2$<br>Ignition Delays<br>Oxidation<br>Shock Tube<br>Stirred Reactor<br>Mechanisms |
| 78915. | Glaude, P.A., V. Warth, R. Fournet, F. Battin-Leclerc, G.M. Come and G. Scacchi, "Modeling of *n*-Heptane and *iso*-Octane Gas Phase Oxidation at Low Temperature by using Computer-Aided Designed Mechanisms," *Bull. Soc. Chim. Belg.* 106, 343-348 (1997). | Kinetic Modeling<br>*n*-$C_7H_{16}$, *i*-$C_8H_{18}/O_2$<br>Automatically Generated Schemes<br>Stirred Reactor<br>Data Comparison |

78916. Doute, C., J.-L. Delfau and C. Vovelle, "Modeling of the Structure of a Premixed *n*-Decane Flame," *Combust. Sci. Technol.* 130, 269-313 (1997).

Kinetic Modeling
$n$-$C_{10}H_{22}/O_2/N_2$
Premixed Flames
Species Profiles
Data Comparisons

78917. Hamiroune, D., P. Bishnu, M. Metghalchi and J.C. Keck, "Rate-Controlled Constrained Equilibrium Method using Constraint Potentials," *Combust. Theory Modeling* 2, 81-94 (1998).

Kinetic Modeling
$H_2$/Air
Reduced Schemes
Method

## 35. PYROLYSIS KINETICS/STUDIES

(78770) Nozzle Expansion, Infrared Laser Jet Spectroscopy, Free Radicals Method, $CH_3$ $\nu_2$ Absorption

Pulse Pyrolysis

(78465) HCN, $NH_3$ , $N_2$ Emission Releases, NaOH, KOH, $Ca(OH)_2$ Seeding Effects

Coal Pyrolysis

(78464) Hydropyrolysis, Effectiveness

Coal/Syngas

78918. Furimsky, E., and Y. Ohtsuka, "Formation of Nitrogen-Containing Compounds during Slow Pyrolysis and Oxidation of Petroleum Coke," *Energy Fuels* 11, 1073-1080 (1997).

Slow Pyrolysis
Petroleum Coke
Oxidation
$HCN, NH_3, NO, N_2O$
Formation
$CaCO_3$ Effects

(78426) Pyrolysis, Gasification, Solar Catalytic, $H_2$ Formation

Biomass

(78423) Pyrolysis, Gasification, Conversions, He, $H_2$ , $CO_2$ , $H_2O$ Additive Effects

Biomass

(78698) Pyrolysis, Alkali Metal Release, Cl Enhancement Effects

Biomass

(78701) Chlorine Release, Gasification

Biomass

78919. Williams, P.T., and E.A. Williams, "Recycling Plastic Waste by Pyrolysis," *J. Inst. Energy* 71, 81-93 (1998).

Pyrolysis
Plastic Wastes
Gas/Oil
Product Analysis
Yields

(78695) Pyrolysis, Melting, Dissociation, Hot Air Jet Incineration

Polyethylene

(78409) Pyrolysis, $C(s) + H_2$ Formation, $H_2 + CO_2$ Conversion to $CH_3OH$

$CH_4$

78920. Huybrechts, G., G. Van Assche and S. van der Auwera, "Kinetics and Mechanism of the Pyrolysis of 1-Chloro-1,1-difluoroethane in the Presence of Additives," *Int. J. Chem. Kinet.* 30, 359-366 (1998).

Pyrolysis
$CF_2ClCH_3$
HCl Elimination
$CCl_4, C_2Cl_6, C_2H_2F_2$
$C_2H_3F_3, HCl$
Additive Effects
Kinetic Modeling

78921. Zhang, Y.-X., C.-L. Yu and S.H. Bauer, "The Pyrolysis of Azetidine: Shock Tube Kinetics Similarities and Contrasts with Two Analogs," *Int. J. Chem. Kinet.* 30, 185-191 (1998).

Pyrolysis
*c*-$(CH_2)_3NH$/Ar
Shock Tube
$(CH_2)_3S$,$(CH_2)_3O$
Kinetic
Thermodynamic
Comparisons

78922. Bauer, S.H., and S. Javanovic, "The Pyrolysis of Octafluorocyclobutane: Revisited," *Int. J. Chem. Kinet.* 30, 171-177 (1998).

Pyrolysis
*c*-$C_4F_8$
High T,P Reactor
Time/Temperature
Calibrator

78923. Zils, R., R. Martin and D. Perrin, "Kinetic Study and Modeling of the Hetero-Homogeneous Pyrolysis and Oxidation of Isobutane around 800 K. II. Pyrolysis in Pyrex Reactors Packed with Platinum Foils or PbO Treated Pyrex Rods," *Int. J. Chem. Kinet.* 30, 439-450 (1998).

Pyrolysis
*i*-$C_4H_{10}$
Pt/PbO Packed
Heated Reactor
H-Atom
Wall Sticking
Coefficients

(78913) Pyrolysis, Self Inhibition, Kinetic Modeling, Data Fitting

*i*-$C_4H_{10}$

(78493) Pyrolysis, Product Yields, Kinetic Parameters

HMX,RDX

(78497) Flash Pyrolysis, Trace Volatiles, Product FTIR

RDX

(78498) Pyrolysis, Unimolecular Rate Constant, Products, Mechanism, Shock Tube

TNAZ

78924. Zegers, E.J.P., and E.M. Fisher, "Gas Phase Pyrolysis of Diisopropyl Methylphosphonate," *Combust. Flame* 115, 230-240 (1998).

Pyrolysis
$CH_3PO_3(i\text{-}C_3H_7)_2$
$CH_3COO(i\text{-}C_3H_7)$
$CH_3COO(t\text{-}C_4H_9)$
Unimolecular
Rate Constants
Product FTIR

(79039) IR Laser Pyrolysis, Rate Constant, Mechanism

$SiH_2Cl_2/SF_6$

78925. Onischuk, A.A., V.P. Strunin, M.A. Ushakova and V.N. Panfilov, "Studying of Silane Thermal Decomposition Mechanism," *Int. J. Chem. Kinet.* 30, 99-110 (1998).

Pyrolysis
$SiH_4$
Flow Reactor
Kinetic Modeling
$Si_2H_6$,Solid Products

## 36. KINETIC MODELING/SENSITIVITIES/RATE CONSTANTS

(See also Section 15 for Ion Reaction Rate Constants, Section 27 for Excited State Rate Constants, Section 35 for Pyrolysis Rate Constants, Section 39 for Unimolecular Rate Constants, Section 40 for Theoretically Calculated Values and Section 45 for Energy Relaxation Rate Constants)

78926. Olcese, L.E., and B.M. Toselli, "Fast and Reliable Numerical Methods to Simulate Complex Chemical Kinetic Mechanisms," *Int. J. Chem. Kinet.* 30, 349-358 (1998).

Kinetic Modeling
Stiff ODE
Integration
Methods

78927. Tadi, M., and R.A. Yetter, "Evaluation of the Rate Constants in Chemical Reactions," *Int. J. Chem. Kinet.* 30, 151-159 (1998).

Rate Constant
Measurements
Extraction
Unknown Values
New Method

78928. Popescu, C., and E. Segal, "Critical Considerations on the Methods for Evaluating Kinetic Parameters from Nonisothermal Experiments," *Int. J. Chem. Kinet.* 30, 313-327 (1998).

Kinetic Parameters
Nonisothermal
Techniques
Analysis
Criteria
Assessments

78929. Smith, M.A., "Low Temperature Rate Studies of Ions and Radicals in Supersonic Flows," *Int. Rev. Phys. Chem.* 17, 35-63 (1998).

$Ar^+ + O_2$
$N_2^+ + N_2 + N_2$
$N_2^+ + O_2$
$OH + HBr$
$OH + NO + N_2$
$O_2^+(v=1) + M$
$NO^+(v=1) + M$
1-200 K
Rate Constants
Review

78930. McDaniel, A.H., and M.D. Allendorf, "Flow Tube Investigation of the High Temperature Reaction between $BCl_3$ and $NH_3$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7804-7812 (1998).

$BCl_3 + NH_3$
Rate Constants
T Dependence
HCl Formation

78931. Burkholder, J.B., "Rate Coefficient for the Reaction: $Br + Br_2O \rightarrow Br_2 + BrO$," *Int. J. Chem. Kinet.* 30, 571-576 (1998).

$Br + Br_2O$
Rate Constant
$Br_2O + h\nu$
Products

78932. Aranda, A., V. Daele, G. Le Bras and G. Poulet, "Kinetics of the Reactions of $CH_3O$ with Br and BrO at 298 K," *Int. J. Chem. Kinet.* 30, 249-255 (1998).

$Br + CH_3O$
$BrO + CH_3O$
Rate Constants

78933. Szilagyi, I., K. Imrik, S. Dobe and T. Berces, "Kinetics of the Reactions of Bromine Atoms with a Series of Aliphatic Aldehydes at 298 K," *Ber. Bunsenges. Phys. Chem.* 102, 79-84 (1998).

Br+RCHO
Rate Constants
$R+CH_3$, $C_2H_5$, $CCl_3$, *i*-$C_3H_7$, *t*-$C_4H_9$
Measurements

78934. Bedjanian, Y., G. Poulet and G. Le Bras, "Low Pressure Study of the Reactions of Br Atoms with Alkenes. I. Reaction with Propene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5867-5875 (1998).

$Br+C_3H_6(+M)$
$C_3H_6Br+Br_2$
$Br+C_3H_5$
Rate Constants
$\Delta H_f(C_3H_6Br)$

78935. Cronkhite, J.M., R.E. Stickel, J.M. Nicovich and P.H. Wine, "Laser Flash Photolysis Studies of Radical-Radical Reaction Kinetics: The $HO_2+BrO$ Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6651-6658 (1998).

$BrO+HO_2$
$HO_2+HO_2$
Rate Constants
Measurements

78936. Behr, P., C. Kaupert, E. Shafranovski and H. Heydtmann, "Temperature Dependence of the Gas Phase Reactions F+CHFO, CFO+F and CFO+CFO," *Int. J. Chem. Kinet.* 30, 329-333 (1998).

CFO+CFO
CFO+F+M
CHFO+F
Rate Constants
T Dependences

78937. Hranisavljevic, J., and J.V. Michael, "Rate Constants for $CF_3+H_2 \rightarrow CF_3H+H$ and $CF_3H+H \rightarrow CF_3+H_2$ Reactions in the Temperature Range 1100-1600 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7668-7673 (1998).

$CF_3+H_2$
$CF_3H+H$
Rate Constants
T Dependences
Equilibrium Constants
Shock Tube

78938. Pagsberg, P., J.T. Jodkowski, E. Ratajczak and A. Sillesen, "Experimental and Theoretical Studies of the Reaction between $CF_3$ and $NO_2$ at 298 K," *Chem. Phys. Lett.* 286, 138-144 (1998).

$CF_3+NO_2$
Rate Constants
$CF_2O$ Product
Branching Ratio
$CF_3$ IR Absorption Coefficient

78939. Rim, K.T., and J.F. Hershberger, "Product Branching Ratios of the $HCO+NO_2$ Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5898-5902 (1998).

$CHO+NO_2$
Branching Ratios
$CO, CO_2, NO$
Product Monitoring

78940. Miller, J.A., C.F. Melius and P. Glarborg, "The $CH_3+NO$ Rate Coefficient at High Temperatures: Theoretical Analysis and Comparison with Experiment," *Int. J. Chem. Kinet.* 30, 223-228 (1998).`

$CH_3+NO$
Rate Constants
Calculation
Shock Tube
Data Comparisons
Branching

78941. Deters, R., M. Otting, H.G. Wagner, F. Temps, B. Laszlo, S. Dobe and T. Berces, "A Direct Investigation of the Reaction $CH_3+OH$: Overall Rate Constant and $CH_2$ Formation at 298 K," *Ber. Bunsenges. Phys. Chem.* 102, 58-72 (1998).

$CH_3+OH(+He)$
Rate Constants
P Dependence
$CH_2$ Product
Branching Ratio

78942. Opeida, I.A., A.F. Dmitruk and O.M. Zarechnaya, "Reactivity of the C-H Bond of Organic Molecules with Various Structures in Hydrogen Abstraction by Peroxyl Radicals," *Theor. Exp. Chem., Russia* 33, 5-10 (1997).

$RO_2+R'H$
H-Abstraction
Activation Energies
Estimation Method

78943. Legrand, J.-C., A.-M. Diamy, R. Hrach and V. Hrachova, "Methane Conversion in the Flowing Afterglow of a Dinitrogen Microwave Plasma: Initiation of the Reaction," *Contrib. Plasma Phys.* 37, 521-537 (1997).

$CH_4/N_2$
Kinetic Modeling
Microwave
Discharge
Products

78944. He, G., I. Tokue, L.B. Harding and R.G. Macdonald, "Thermal Rate Constant and Branching Ratio for $CN+HD \rightarrow HCN/DCN+D/H$ from 293 to 375 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7653-7661 (1998).

$CN+HD$
Rate Constants
Branching Ratio
HCN,DCN Products

78945. Klippenstein, S.J., D.L. Yang, T. Yu, S. Kristyan, M.C. Lin and S.H. Robertson, "A Theoretical and Experimental Study of the $CN+NO$ Association Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6973-6980 (1998).

$CN+NO(+M)$
Rate Constants
P,T Dependences
Measurements
RRKM Analysis
Data Fitting

78946. Czarnowski, J., "Kinetics and Mechanism of the Thermal Gas Phase Oxidation of Tetrachloroethene by Molecular Oxygen in Presence of Trifluoromethylhypofluorite, $CF_3OF$," *Z. Phys. Chem. (Munchen)* 203, 183-197 (1998).

$C_2Cl_4/O_2/CF_3OF$
Chain Reaction
Mechanism
Products
Rate Constants

78947. Hasson, A.S., C.M. Moore and I.W.M. Smith, "The Fluorine Atom Initiated Oxidation of $CF_3CFH_2$ (HFC-134a) Studied by FTIR Spectroscopy," *Int. J. Chem. Kinet.* 30, 541-554 (1998).

$CF_3CFH_2/O_2/F$
Oxidation
$CF_3CFHO+O_2$,M
Relative
Rate Constants
Product Yields

78948. Herbst, E., and D.E. Woon, "The Rate of the Reaction between $C_2H$ and $C_2H_2$ at Interstellar Temperatures," *Astrophys. J.* 489, 109-112 (1997).

$C_2H+C_2H_2$
Rate Constants
10-300 K
$C_4H_2$ Product
Calculations

78949. Hoobler, R.J., and S.R. Leone, "Rate Coefficients for Reactions of Ethynyl Radical ($C_2H$) with HCN and $CH_3CN$: Implications for the Formation of Complex Nitriles on Titan," *J. Geophys. Res.* 102, 28717-28723 (1997).

$C_2H+CH_3CN$
$C_2H+HCN$
Rate Constants
T Dependences

78950. Lifshitz, A., and C. Tamburu, "Thermal Decomposition of Acetonitrile: Kinetic Modeling," *Int. J. Chem. Kinet.* 30, 341-347 (1998).

$CH_3CN$
Thermal Dissociation
Kinetic Modeling
Data Comparison

(78895) Rate Constants, $C_2H_4/O_2/Ar$ Flames, Molecular Beam/Mass Analysis, Species Profiles

$C_2H_4 + H,OH$
$C_2H_3 \rightarrow$

(79223) Rate Constants, Temperature Dependences, $\Delta H_f(C_2H_5, C_2H_4Cl)$, $D(C_2H_5Cl, C_3H_7Cl, C_2H_4Cl_2)$, Measurements

$C_2H_5 + HBr$
$C_2H_4Cl + HBr$

78951. Dilger, H., M. Stolmar, U. Himmer, E. Roduner and I.D. Reid, "Kinetics of the Gas Phase Addition of the Ethyl Radical and the *tert*-Butyl Radical to NO," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6772-6777 (1998).

$C_2H_5 + NO$
$t\text{-}C_4H_9 + NO$
Rate Constants
T Dependences
Muonium Labeling Method

78952. Curran, H.J., W.J. Pitz, C.K. Westbrook, P. Dagaut, J.-C. Boettner and M. Cathonnet, "A Wide Range Modeling Study of Dimethyl Ether Oxidation," *Int. J. Chem. Kinet.* 30, 229-241 (1998).

$(CH_3)_2O/O_2$
Kinetic Modeling
Stirred Reactor
Shock Tube
Data Comparisons

78953. Aschmann, S.M., and R. Atkinson, "Kinetics of the Gas Phase Reactions of the OH Radical with Selected Glycol Ethers, Glycols and Alcohols," *Int. J. Chem. Kinet.* 30, 533-540 (1998).

$C_3H_6(OH)_2 + OH$
$(CH_3O)C_3H_6OH + OH$
$CH_3CH(OC_4H_9)OH + OH$
$C_6H_{13}OH, C_2H_4(OH)_2 + OH$
$(CH_3O)C_3H_6OH + NO_3, O_3$
$CH_3CH(OC_4H_9)OH + NO_3, O_3$
Rate Constants
Atmospheric Lifetimes

78954. Sehested, J., L.K. Christensen, O.J. Nielsen, M. Bilde, T.J. Wallington, W.F. Schneider, J.J. Orlando, G.S. Tyndall, "Atmospheric Chemistry of Acetone: Kinetic Study of the $CH_3C(O)CH_2O_2 + NO/NO_2$ Reactions and Decomposition of $CH_3C(O)CH_2O_2NO_2$," *Int. J. Chem. Kinet.* 30, 475-489 (1998).

$CH_3COCH_2 + NO, NO_2$
$CH_3COCH_2O_2 + NO$
$CH_3COCH_2O_2 + NO_2$
Rate Constants
$CH_3COCH_2O_2NO_2 \rightarrow$
IR Spectrum
Dissociation Rate

78955. Friedrichs, G., H.G. Wagner, "Investigation of the Thermal Decay of Carbon Suboxide," *Z. Phys. Chem. (Munchen)* 203, 1-14 (1998).

$C_3O_2 + M$
$C_3O_2 + C$
Rate Constants
T Dependences
$C_2O + M$
Energy Barrier
$\Delta H_f(C_2O)$
Shock Tube

78956. Fantechi, G., N.R. Jensen, J. Hjorth and J. Peeters, "Determination of the Rate Constants for the Gas Phase Reactions of Methyl Butenol with OH Radicals, Ozone, $NO_3$ Radicals and Cl Atoms," *Int. J. Chem. Kinet.* 30, 589-594 (1998).

$(CH_3)_2C(OH)CHCH_2+M$
$M=OH,O_3,NO_3,Cl$
Rate Constants
Atmospheric Lifetimes

78957. Platz, J., O.J. Nielsen, T.J. Wallington, J.C. Ball, M.D. Hurley, A.M. Straccia, W.F. Schneider and J. Sehested, "Atmospheric Chemistry of the Phenoxy Radical, $C_6H_5O$: Ultraviolet Spectrum and Kinetics of Its Reaction with NO, $NO_2$ and $O_2$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7964-7974 (1998).

$C_6H_5O+NO,NO_2$
$C_6H_5O+O_2$
$C_6H_5OH+Cl,Cl_2$
$ClC_6H_5OH+Cl$
Benzoquinone+Cl
Rate Constants
$C_6H_5O$
UV Absorption Cross Sections

78958. Berho, F., and R. Lesclaux, "The Phenoxy Radical: Ultraviolet Spectrum and Kinetics of Gas Phase Reactions with Itself and with Oxygen," *Chem. Phys. Lett.* 279, 289-296 (1997).

$C_6H_5O+O_2$
$C_6H_5O+C_6H_5O$
Rate Constants
T Dependences
$C_6H_5O$
UV Absorption Cross Sections

78959. Kaiser, E.W., and T.J. Wallington, "Comment on the Inverse Kinetic Isotope Effect in the Reaction of Atomic Chlorine with $C_2H_4$ and $C_2D_4$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6054-6055 (1998).

$Cl+C_2H_4+M$
Rate Constants
$M=He,N_2$
Pressure,M Effects

78960. Stutz, J., M.J. Ezell and B.J. Finlayson-Pitts, "Reply to the Comment on the Inverse Kinetic Isotope Effect in the Reaction of Atomic Chlorine with $C_2H_4$ and $C_2D_4$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6056 (1998).

Reply

78961. Wallington, T.J., A. Guschin and M.D. Hurley, "Comment on a Kinetic Study of Chlorine Radical Reactions with Ketones by Laser Photolysis Technique by Olsson et al.," *Int. J. Chem. Kinet.* 30, 309-310 (1998).

$Cl+c\text{-}C_5H_8O$
$Cl+c\text{-}C_6H_{10}O$
Rate Constants
Relative to
$c\text{-}C_5H_{10}$, $c\text{-}C_6H_{12}$
$C_2H_4$
Comments

78962. Ljungstrom, E., and M. Hallquist, "Reply to Comment by Wallington et al.," *Int. J. Chem. Kinet.* 30, 311 (1998).

Reply

(78838) (78839) Rate Constant, NCl(a) Product Branching Ratio

$Cl+N_3$

78963. Louis, F., and J.-P. Sawerysyn, "Kinetics and Products Studies of Reactions between Fluorine Atoms and $CHF_3$, $CHClF_2$, $CHCl_2F$ and $CHCl_3$," *J. Chem. Soc., Faraday Trans.* 94, 1437-1445 (1998).

$F+CHF_3,CHClF_2$
$F+CHCl_2F,CHCl_3$
Rate Constants
T Dependences

78964. Eichholtz, M., A. Schneider, J.-T. Vollmer and H.G. Wagner, "Kinetic Investigations of the Reactions of Tetramethylgermane, Tetraethylgermane, Tetramethoxygermane and 3,3-Diethylpentane with O($^3$P) Atoms," *Z. Phys. Chem. (Munchen)* 199, 267-274 (1997).

$Ge(CH_3)_4 + O$
$Ge(C_2H_5)_4 + O$
$Ge(OCH_3)_4 + O$
$C_9H_{20} + O$
Rate Constants
T Dependences

(79019) Cross Sections, OH($^2\Pi_{1/2}$, v=0,N=1), $H_2$ Product Energy Distributions, Measurements

Hot 'H' + $H_2O$

78965. Bohn, B., and C. Zetzsch, "Formation of $HO_2$ from OH and $C_2H_2$ in the Presence of $O_2$," *J. Chem. Soc., Faraday Trans.* 94, 1203-1210 (1998).

$HO_2 + CO, C_2H_2$
$HO_2 + NO$
$OH + CO, NO$
Rate Constants
$C_2H_2/O_2/NO$
$OH, HO_2$
Formation Yields

(78514) Rate Constant Assessments, $H_2/O_2$ Auto-ignition, Higher Pressures

$H_2O_2 + H$

78966. Payne, W.A., R.P. Thorn Jr, F.L. Nesbitt and L.J. Stief, "Rate Constant for the Reaction of O($^3$P) with IO at 298 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6247-6250 (1998).

IO + O
Rate Constant
Measurement

78967. Kind, I., T. Berndt and O. Boge, "Gas Phase Rate Constants for the Reaction of $NO_3$ Radicals with a Series of Cyclic Alkenes, 2-Ethyl-1-butene and 2,3-Dimethyl-1,3-butadiene," *Chem. Phys. Lett.* 288, 111-118 (1998).

$NO_3$ + *c*-Alkenes
$NO_3 + C_5H_{10}, C_6H_{10}$
Rate Constants
16 Reactions
Measurements

78968. Chew, A.A., R. Atkinson and S.M. Aschmann, "Kinetics of the Gas Phase Reactions of $NO_3$ Radicals with a Series of Alcohols, Glycol Ethers, Ethers and Chloroalkenes," *J. Chem. Soc., Faraday Trans.* 94, 1083-1089 (1998).

$NO_3 + ROR'$
$NO_3 + ROR'OH$
$NO_3 + ROH$
$NO_3$ + Chloroalkenes
Rate Constants
17 Reactions
Products

78969. Hewett, K.B., and D.W. Setzer, "Chemical Kinetics of the Azide Radical: Rate Constants for Reactions with Cl, NO, $NO_2$, $O_2$, CO, $CO_2$, $Cl_2$ and $C_3H_6$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6274-6281 (1998).

$N_3 + F, Cl, NO, N_3$
$N_3 + CO, CO_2, Cl_2$
$N_3 + NO_2, O_2, C_3H_6$
Rate Constants
Measurements

78970. Coeur, C., V. Jacob, P. Foster and P. Baussand, "Rate Constant for the Gas Phase Reaction of Hydroxyl Radical with the Natural Hydrocarbon Bornyl Acetate," *Int. J. Chem. Kinet.* 30, 497-502 (1998).

OH + Bornyl Acetate
Rate Constant

78971. Aschmann, S.M., and R. Atkinson, "Rate Constants for the Gas Phase Reactions of Selected Dibasic Esters with the OH Radical," *Int. J. Chem. Kinet.* 30, 471-474 (1998).

OH + Esters
Rate Constants
$(CH_2COOCH_3)_2$
$CH_2(CH_2COOCH_3)_2$
$(CH_2CH_2COOCH_3)_2$
Atmospheric Lifetimes

78972. Arthur, N.L., and L.A. Miles, "Arrhenius Parameters for $H + (CH_3)_{4-n}SiH_n$, n=1-3," *J. Chem. Soc., Faraday Trans.* 94, 1077-1081 (1998).

$Si(CH_3)H_3 + H$
$Si(CH_3)_2H_2 + H$
$Si(CH_3)_3H + H$
Rate Constants
T Dependences

78973. Kunz, A., and P. Roth, "A High Temperature Study of the Reaction $SiH_4 + H \leftrightarrow SiH_3 + H_2$," *Ber. Bunsenges. Phys. Chem.* 102, 73-78 (1998).

$SiH_4 + H$
Rate Constant
T Dependence
Shock Tube

## 37. PHOTOLYSIS/MPD

(See also Section 38 for Photolytic Product Distributions)

(78931) Photolysis Products, $Br + Br_2O$ Rate Constant

$Br_2O + h\nu$

78974. Radloff, W., P. Farmanara, V. Stert, E. Schreiber and J.R. Huber, "Ultrafast Photodissociation Dynamics of Electronically Excited $CF_2I_2$ Molecules," *Chem. Phys. Lett.* 291, 173-178 (1998).

$CF_2I_2 + h\nu$
fs Pump/Probe
Concerted Dissociation

78975. Hechtfischer, U., Z. Amitay, P. Forck, M. Lange, J. Linkemann, M. Schmitt, U. Schramm, D. Schwalm, R. Wester, D. Zajfman and A. Wolf, "Near-Threshold Photodissociation of Cold $CH^+$ in a Storage Ring," *Phys. Rev. Lett.* 80, 2809-2812 (1998).

$CH^+ + h\nu$
$C^+(^2P_{1/2,3/2})$
Product Resonances

78976. Lundell, J., M. Krajewska and M. Rasanen, "Matrix Isolation Fourier Transform Infrared and ab Initio Studies of the 193 nm Induced Photodecomposition of Formamide," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6643-6650 (1998).

$CH(O)NH_2 + h\nu$
Product FTIR
Ar,Xe Matrix Studies

78977. Lim, S.-M., T.-S. Kim, G.-I. Lim, S.K. Kim and Y.S. Choi, "Direct Formation of $CH_2(b^1B_1)$ in the Near-Ultraviolet Photodissociation of Diazirine," *Chem. Phys. Lett.* 288, 828-832 (1998).

$CH_2N_2 + h\nu$
$CH_2$(b,v) Product Emission Decays

78978. Lee, Y.-J., Y.-R. Lee, C.-C. Chou and S.-M. Lin, "The C-Cl Bond Fissions from the Photolysis of $CHCl=CCl_2$ at 193 nm," *J. Chem. Phys.* 109, 346-347 (1998).

$C_2Cl_3 + h\nu$
Fragment Energies
Channels
Mechanism

78979. Quandt, R., X. Wang, Z. Min, H.L. Kim and R. Bersohn, "One-Color Molecular Photodissociation and Detection of Hydrogen Atoms," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6063-6067 (1998).

$C_2H_3$,$C_3H_5$+hν
HCOOH,$H_2S$+hν
205.1 nm
Photolysis
Simultaneous
2-Photon
H-Atom LIF
H Product Energies

(78779) Photofragment Products, Cross Sections

$CH_3CO_2I^-$+hν

78980. Chang, A.H.H., A.M. Mebel, X.-M. Yang, S.H. Lin and Y.T. Lee, "Ab Initio Calculations of Potential Energy Surface and Rate Constants for Ethylene Photodissociation at 193 and 157 nm," *Chem. Phys. Lett.* 287, 301-306 (1998).

$C_2H_4$+hν
Rate Constants
Channels
RRKM Theory

78981. Chang, A.H.H., A.M. Mebel, X.-M. Yang, S.H. Lin and Y.T. Lee, "Ab Initio/RRKM Approach Toward the Understanding of Ethylene Photodissociation," *J. Chem. Phys.* 109, 2748-2761 (1998).

$C_2H_4$+hν(VUV)
D-Isotopes
Channels
RRKM Analysis
Rate Constants

78982. Lin, J.J., D.W. Hwang, Y.T. Lee and X. Yang, "Site and Isotope Effects on the Molecular Hydrogen Elimination from Ethylene at 157 nm Excitation," *J. Chem. Phys.* 109, 2979-2982 (1998).

$C_2H_4$+hν(157 nm)
$H_2$ Elimination
Channels
D Labeling
Mechanisms

78983. Koda, S., T. Ebukuro, J. Otomo, T. Tsuruno and Y. Oshima, "Photooxidation Reactions of Ethylene in Supercritical $CO_2$," *J. Photochem. Photobiol. A. Chem.* 115, 7-11 (1998).

$C_2H_4/O_2/CO_2$
Supercritical
Conditions
Photooxidation
Main Products
Quantum Yields

78984. Lim, S.-H., J.C. Choe and M.S. Kim, "$C_6H_5Br^+ \rightarrow C_6H_5^+ + Br$ Occurs via Orbiting Transition State," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7375-7381 (1998).

$C_6H_5Br^+$+hν
Rate Constant
Energy Release
RRKM Model

78985. Wang, G.-J., R.-S. Zhu, H. Zhang, K.-L. Han, G.-Z. He and N.-Q. Lou, "Photodissociation of Chlorobenzene at 266 nm," *Chem. Phys. Lett.* 288, 429-432 (1998).

$C_6H_5Cl$+hν
Cl Fragment
Energies
Mechanism

78986. Christophy, E., K. Myli, T.R. Viegut, J.A. Rzepiela and J.M. Hossenlopp, "Detection of Benzaldehyde and Formaldehyde in the Ultraviolet Photolysis of Gas Phase Methyl Benzoate," *J. Photochem. Photobiol. A. Chem.* 110, 229-234 (1997).

$C_6H_5COOCH_3$+hν
Product
Phosphorescence
$C_6H_5CHO^*$,$HCHO^*$
$CH_2O^*/CH_2O$ Ratio

78987. Hwang, W.G., J.H. Moon, J.C. Choe and M.S. Kim, "Dissociation Dynamics of *n*-Propylbenzene Molecular Ion," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7512-7518 (1998).

$C_6H_5(n\text{-}C_3H_7^+)+h\nu$
$C_7H_7^+$ Product
Mass Analysis
Rate Constants
Dynamics

78988. Sorokin, V.I., and A.I. Chichinin, "The 248 nm Photodissociation of $ClF_3$: Quantum Yields for F and Cl Atoms," *Chem. Phys. Lett.* 280, 141-144 (1997).

$ClF_3+h\nu$
F,Cl Product
Quantum Yields
$ClF_2+F$
Primary Step

78989. Kreher, C.J., R.T. Carter and J.R. Huber, "Vector Correlations in the Photodissociation of $OClO(A^2A_2(\nu_1,0,0))$," *Chem. Phys. Lett.* 286, 389-397 (1998).

$ClO_2(A\text{-}X)$
Photodissociation
$ClO(v=0)$
Product Angular
Correlations
Channels

78990. Delmdahl, R.F., S. Ullrich and K.-H. Gericke, "Photofragmentation of $OClO(A^2A_2,\nu_1\nu_2\nu_3)\rightarrow Cl(^2P_J)+O_2$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7680-7685 (1998).

$ClO_2+h\nu$
360-450 nm
ClO,Cl Channels
Branching Ratio
Quantum Yields

78991. Fioretti, A., D. Comparat, A. Crubellier, O. Dulieu, F. Masnou-Seeuws and P. Pillet, "Formation of Cold $Cs_2$ Molecules through Photodissociation," *Phys. Rev. Lett.* 80, 4402-4405 (1998).

$Cs+Cs+h\nu$
Photoassociation
$Cs_2(^3\Sigma_u^+)$
Formation
Cold Trap

(78744) IR MPD, $Fe_2O_3$ Nanoparticle Formation, Sizes

$Fe(CO)_5/SF_6$

(79119) P.E. Surfaces, Fitting Process, Cross Section, Calculations

$HCl^+ + h\nu$

(79106) Laser Control, Autoionization, Predissociation, $HI^+$, $I^+$ Phase Lags

$HI,DI+h\nu$

78992. Pehkonen, S., M. Pettersson, J. Lundell, L. Khriachtchev and M. Rasanen, "Photochemical Studies of Hydrogen Peroxide in Solid Rare Gases: Formation of the $HOH\cdots O(^3P)$ Complex," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7643-7648 (1998).

$H_2O_2+h\nu$
Matrix Study
$OH,H_2O.O$
Products
FTIR Spectra

78993. Franks, K.J., H. Li, R.J. Hanson and W. Kong, "Selective Excitation of ICN Achieved via Brute Force Orientation," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7881-7884 (1998).

$ICN+h\nu$
Orientated
Molecules
Polarized Laser
CN(J) Product
Effects

78994. Paniagua, M., A. Aguado, M. Lara and O. Roncero, "Transition State Spectroscopy on the Li-HF System," *J. Chem. Phys.* 109, 2971-2974 (1998).

Li.HF + hν
Photoinitiation
Absorption Spectrum
LiF Product
Mechanism

78995. Lu, Y., W.C. Stolte and J.A.R. Samson, "Kinetic Energy Study of the Ion Fragments Produced by Dissociative Photoionization of Nitric Oxide," *J. Electron Spectrosc. Relat. Phenom.* 87, 109-120 (1997).

NO + hν
Photoionization
19-60 eV
$N^+$,$O^+$ Fragments
Mechanisms

78996. Dietz, H., and V. Engel, "Pump/Probe Spectroscopy of NaI in Rare Gas Environments: A Statistical Description," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7406-7413 (1998).

NaI/Rg + hν
fs Pump/Probe
Predissociation
Dynamics
Theory

(78621) Above Threshold Dissociation Channels, Na(3p) Product

$Na_2^+ + 2h\nu$

78997. Lin, J.J., D.W. Hwang, Y.T. Lee and X. Yang, "Photodissociation of $O_2$ at 157 nm: Experimental Observation of Anisotropy Mixing in the $O_2 + h\nu \rightarrow O(^3P) + O(^3P)$ Channel," *J. Chem. Phys.* 109, 1758-1762 (1998).

$O_2 + h\nu$(157 nm)
Branching Ratio
$O(^1D,^3P)$
Product Channels
Anisotropy
Parameters

78998. Ravishankara, A.R., G. Hancock, M. Kawasaki and Y. Matsumi, "Photochemistry of Ozone: Surprises and Recent Lessons," *Science* 280, 60-61 (1998).

$O_3 + h\nu$
$O(^1D)$ Formation
Quantum Yields
Tail Contributions

78999. Patzer, S., N.L. Arthur, P. Potzinger and H.G. Wagner, "Photolysis of Hexamethyldisilane at 206 nm," *J. Photochem. Photobiol. A. Chem.* 110, 221-227 (1997).

$Si_2(CH_3)_6 + h\nu$
Product Channels
Quantum Yields
Mechanisms

79000. Parthasarathy, V., S. Nad, K.A. Rao and S.K. Sarkar, "Intensity and Pressure Effects in $CO_2$ Laser Induced Carbon-13 Enrichment with Temporally Modified Pulses," *J. Photochem. Photobiol. A. Chem.* 115, 1-6 (1998).

IR MPD
$CF_2HCl$
$^{13}C$ Enrichment
Modified Pulse
Effects

79001. Petrov, A.K., E.N. Chesnokov, S.R. Gorelik, Yu.N. Molin, K.D. Straub, J.M.J. Madey and E.B. Szarmes, "Isotope-Selective Infrared Multiphoton Dissociation of Formic Acid with a Free Electron Laser," *Dokl. Phys. Chem.* 352, 72-74 (1997).

IR MPD
HCOOH
$\nu_{CO}$,$\nu_{CH}$
Frequencies
Isotopic
Selectivity
Product Yields

(79183) IR Laser Excitation/Thermal Lensing Monitor of Vibrational Relaxation Rates Compared to IR MPD Corresponding Processes

IR MPD
$CClF_2CHCl_2$

79002. Pushpa, K.K., A. Kumar, P.D. Naik, K.A. Rao, V. Parthasarathy, S.K. Sarkar and J.P. Mittal, "Visible Luminescence Studies in the Infrared Multiphoton Dissociation of 1,2-Dichloro-1,1-difluoroethane," *Chem. Phys. Lett.* 279, 172-178 (1997).

IR MPD
$C_2H_2Cl_2F_2$
Visible Luminescence
$CF_2ClCH$
Assignment

79003. Dem'yanenko, A.V., E.A. Ryabov and V.S. Letokhov, "Infrared Multiphoton Dissociation of $Br(CF_2)_4COI$ Molecules by Excitation via C=O (1794 $cm^{-1}$) Stretching and Skeleton (961 $cm^{-1}$) Vibrations," *Chem. Phys. Lett.* 286, 277-283 (1998).

IR MPD
$Br(CF_2)_4COI$
Products
Laser Frequency Effects

(79187) Vibrational Relaxation, 14500-17500 $cm^{-1}$ Energies, Compared to Ultraviolet Pumping (40300 $cm^{-1}$), Agreements

IR MPA,$C_6F_6$

79004. von Helden, G., I. Holleman, A.J.A. van Roij, G.M.H. Knippels, A.F.G. van der Meer and G. Meijer, "Shedding New Light on Thermionic Electron Emission of Fullerenes," *Phys. Rev. Lett.* 81, 1825-1828 (1998).

IR MPA/MPI
$C_{60}$
Autoionization Rates
Electronically Excited State Roles

79005. Ihee, H., J. Cao and A.H. Zewail, "Ultrafast Electron Diffraction: Structures in Dissociation Dynamics of $Fe(CO)_5$," *Chem. Phys. Lett.* 281, 10-19 (1997).

UV MPD
$Fe(CO)_5$
Fe,FeCO,$Fe(CO)_2$
Products
Fast Electron Diffraction Monitor

## 38. REACTION PRODUCT-ENERGY DISTRIBUTIONS

(See also Section 37 for Product Distributions and Section 40 for Theoretically Calculated Reaction Product Distributions)

79006. Jee, Y.-J., M.S. Park, Y.S. Kim, Y.-J. Jung and K.-H. Jung, "Photodissociation of Bromine Molecule Near 265 nm," *Chem. Phys. Lett.* 287, 701-708 (1998).

$Br(^2P_{1/2,3/2})$
Energy, Angular Distributions
$Br_2+h\nu$
Mechanism

79007. Scholefield, M.R., J.-H. Choi, S. Goyal and H. Reisler, "Endoergic Reactions of Hyperthermal $C(^3P)$ with Methane and Acetylene," *Chem. Phys. Lett.* 288, 487-493 (1998).

CH
Product Energies
'Hot' $C+CH_4$
'Hot' $C+C_2H_2$
Mechanisms

| | | |
|---|---|---|
| (78828) | Product Distribution, $Ar(^3P_{2,0}) + NaCN$, KCN, RbCN, Mechanism | CN(B,v) |
| 79008. | Tomashevsky, M., E. Herbst and W.P. Kraemer, "Classical and Quantum Mechanical Calculations of $HCO^+ + e \rightarrow CO(v) + H$," *Astrophys. J.* 498, 728-734 (1998). | CO(a,X),v<br>Product Distributions<br>$HCO^+ + e^-$<br>Calculations |
| 79009. | Castillejo, M., S. Couris, E. Lane, M. Martin and J. Ruiz, "Laser Photodissociation of Ketene at 230 nm," *Chem. Phys.* 232, 353-360 (1998). | CO(v,J)<br>Product State Distribution<br>$CH_2CO + h\nu$<br>Channels |
| 79010. | Bracker, A.S., E.R. Wouters, A.G. Suits, Y.T. Lee and O.S. Vasyutinskii, "Observation of Coherent and Incoherent Dissociation Mechanisms in the Angular Distribution of Atomic Photofragment Alignment," *Phys. Rev. Lett.* 80, 1626-1629 (1998). | Cl<br>Product Angular Alignment<br>$Cl_2 + h\nu$<br>Ion Imaging<br>State Symmetries<br>Coherence Effects |
| 79011. | Tanaka, Y., M. Kawasaki, Y. Matsumi, H. Fujiwara, T. Ishiwata, L.J. Rogers, R.N. Dixon and M.N.R. Ashfold, "The Ultraviolet Photodissociation of $Cl_2O$ at 235 nm and of HOCl at 235 and 266 nm," *J. Chem. Phys.* 109, 1315-1323 (1998). | $Cl(^2P_{1/2,3/2})$<br>Product Energy Angular Distributions<br>$Cl_2O + h\nu$<br>$HOCl + h\nu$<br>Ion Imaging Method |
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$H_2O$,HOD(v)
Product Energy Distributions
$CH_3SH + OH,OD$
$(CH_3)_2S + OH,OD$
$H_2S + OH,OD$
NO(v=1) From Secondary Reactions
S-Radicals/$NO_2$,NO

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$I(^2P_{1/2,3/2})$
Photofragments
$CF_2I_2 + h\nu$(ns)
Branching Ratios
Channels
REMPI/TOF

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NH(a,X),v,J
Product Energies
Branching Ratios
$HNCO(3\nu_{NH}) + h\nu$
Reactant Excitation Effects

79017. Kennedy, G.R., C.-L. Ning and J. Pfab, "The 355 nm Photodissociation of Jet Cooled $CH_3SNO$: Alignment of the NO Photofragment," *Chem. Phys. Lett.* 292, 161-166 (1998).

NO(v=0,1,J)
Fragment Alignment
$CH_3SNO + h\nu$
Jet Cooled

(78650) (78651) Desorbed Energies, Heterogeneous N-Atom Recombination on Cu

$N_2$(T,v,J)

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OH(X,v,J)
Product Energy Distributions
$t\text{-}C_4H_9OOH + h\nu$
DFWM Monitor Dynamics

79019. Brouard, M., I. Burak, G.A.J. Markillie, K. McGrath and C. Vallance, "The $H + H_2O \rightarrow OH + H_2$ Reaction: OH State-Resolved Differential Cross Sections and $H_2$ Internal Energy Disposals," *Chem. Phys. Lett.* 281, 97-104 (1997).

$OH(^2\Pi_{1/2},v=0,N=1),H_2$
Product Energy Distributions
Hot 'H' + $H_2O$
Cross Sections
Measurements

79020. Brouard, M., I. Burak, S.D. Gatenby and G.A.J. Markillie, "The Product State-Resolved Dynamics of the Reaction $H + N_2O \rightarrow OH(v',j') + N_2$," *Chem. Phys. Lett.* 287, 682-688 (1998).

OH(T,v,J),$N_2$
Product Energy Distributions
$H + N_2O$
1.48 eV Energy

79021. Flothmann, H., R. Schinke, C. Woywod and W. Domcke, "Photodissociation of Ozone in the Chappuis Band. III. Product State Distributions," *J. Chem. Phys.* 109, 2680-2684 (1998).

$O_2(v,J)$
Product State Distributions
$O_3 + h\nu$
(16500 $cm^{-1}$ Band)
Calculations

79022. Zhan, J.-P., H.-P. Yang, K.-L. Han, M.-L. Wang, W.-Q. Deng, G.-Z. He and N.-Q. Lou, "Rotational Alignment of Products from NOCl+Sr Chemiluminescent Reaction," *J. Chem. Phys.* 109, 1819-1823 (1998).

SrCl(B,A)
Vibrational Distributions
Branching Ratio
Rotational Alignment
Sr + NOCl

(78627) Product Branching Ratios, $Xe^+(^2P_{1/2,3/2}) + Cl^- + He$ Reactions, Mechanisms

XeBr(B,D)
$Xe(^3P_1, ^1D_2), Br(^2P_{1/2})$

## 39. UNIMOLECULAR PROCESSES

(See also Section 36 for Unimolecular Rate Constants, Section 37 for Photolytic Systems and Section 40 for Reaction Dynamics)

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Unimolecular Reaction Rate Theory
Semiclassical Quantum Derivation

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Unimolecular Dissociation
Ion Clusters
Blackbody Radiative Initiation
Evidence

79025. Schinke, R., C. Beck, S.Yu. Grebenshchikov and H.-M. Keller, "Unimolecular Dissociation: A State-Specific Quantum Mechanical Perspective," *Ber. Bunsenges. Phys. Chem.* 102, 593-611 (1998).

Unimolecular Dissociation
HCO,HNO
TST
Review

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Unimolecular Dissociation
HC(O)SH
Channels
Energies
Transition States

| | | |
|---|---|---|
| 79027. | Ishikawa, H., C. Nagao, N. Mikami and R.W. Field, "Spectroscopic Investigation of the Generation of 'Isomerization' States: Eigenvector Analysis of the Bend-CP Stretch Polyad," *J. Chem. Phys.* 109, 492-503 (1998). | Isomerization<br>HCP/CPH<br>Highly Excited Vibrational Levels<br>Polyad Model |
| 79028. | Abou-Zied, O.K., and J.D. McDonald, "Picosecond Real Time Study of the Bimolecular Reaction of $O(^3P)+C_2H_4$ and the Unimolecular Photodissociation of $CH_3CHO$ and $H_2CO$," *J. Chem. Phys.* 109, 1293-1301 (1998). | $CH_2O+h\nu$<br>$CH_3CHO+h\nu$<br>$C_2H_4.NO_2+h\nu$<br>ps Pump/Probe<br>REMPI/LIF<br>Product Monitors<br>Dynamics<br>RRKM Analysis |
| 79029. | Germann, T.C., and W.H. Miller, "Quantum Mechanical Calculation of Resonance Tunneling in Acetylene Isomerization via the Vinylidene Intermediate," *J. Chem. Phys.* 109, 94-101 (1998). | Isomerization<br>$^{13}CDCH/^{13}CHCD$<br>Rate Constants<br>Calculations |
| (79013) | Unimolecular Dissociations, HCl(v), CO(v) Product Distributions | $CH_3COCl^*$<br>$CH_2FCOCl^*$ |
| 79030. | Wang, D., and X. Qian, "Determination of the Kinetic Parameters of the Isomerization Reaction of Ethyl Isocyanide using He(I) Photoelectron Spectroscopy," *J. Electron Spectrosc. Relat. Phenom.* 83, 41-44 (1997). | Isomerization<br>$C_2H_5NC/C_2H_5CN$<br>Rate Constants<br>Activation Energy |
| (79224) | Isomerization Energies, Calculations | $HCNCN^+/CNCNH^+$ |
| 79031. | Dubnikova, F., and A. Lifshitz, "Isomerization of Cyclopropanecarbonitrile: Quantum Chemical and Model Calculations," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5876-5885 (1998). | Isomerization<br>*c*-$C_3H_5CN$<br>Channels<br>Major Products<br>Mechanisms |
| 79032. | Fulle, D., A. Dib, J.H. Kiefer, Q. Zhang, J. Yao and R.D. Kern, "Pyrolysis of Furan at Low Pressures: Vibrational Relaxation, Unimolecular Dissociation and Incubation Times," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7480-7486 (1998). | Unimolecular Dissociation<br>*c*-$C_4H_4O$/Ne,Kr<br>Vibrational Relaxation<br>Rate Constants<br>Shock Tube |
| (79150) | Isomerizations, Isomers, Geometries, Frequencies, Energies, Structural Calculations | $CH_2CHCHCH$ |

79033. Deng, W.-Q., K.-L. Han, J.-P. Zhan and G.-Z. He, "Ab Initio and RRKM Calculations of *o*-Benzyne Pyrolysis," *Chem. Phys. Lett.* 288, 33-36 (1998).

Unimolecular Dissociation
*o*-$C_6H_4$
RRKM
Rate Constants
Products

(78924) Unimolecular Rate Constants, Pyrolysis, Product FTIR

$CH_3COO(i\text{-}C_3H_7)$
$CH_3COO(t\text{-}C_4H_9)$
$CH_3PO_3(i\text{-}C_3H_7)_2$

(78610) Isomerization, Dissociation, Photoionization, Ion Fragmentation Efficiencies, Review

Aromatic Hydrocarbons

79034. Leitner, D.M., and P.G. Wolynes, "Quantum Energy Flow during Molecular Isomerization," *Chem. Phys. Lett.* 280, 411-418 (1997).

Isomerization
*trans/cis*$(C_6H_5CH)_2$
Energy Flow
Model

(78498) Pyrolysis, Unimolecular Rate Constant, Products, Mechanism, Shock Tube

TNAZ

79035. Krokidis, X., B. Silvi and M.E. Alikhani, "Topological Characterization of the Isomerization Mechanisms in XNO(X=H,Cl)," *Chem. Phys. Lett.* 292, 35-45 (1998).

Isomerization
ClNO/ClON
HNO/NOH
Mechanism
Theory

79036. Hansel, A., M. Glantschnig, C. Scheiring, W. Lindinger and E.E. Ferguson, "Energy Dependence of the Isomerization of $HCN^+$ to $HNC^+$ via Ion Molecule Reactions," *J. Chem. Phys.* 109, 1743-1747 (1998).

Isomerization
$HCN^+/HNC^+$
Reaction Catalyzed
$CO,CO_2$ Induced
Collision Energy
Effects

79037. Chan, W.-T., and I.P. Hamilton, "Improved Potential Function for $HOO^-/OOH^-$ Isomerization," *Chem. Phys. Lett.* 292, 57-62 (1998).

Isomerization
$HOO^-/OOH^-$
P.E. Surface
Fitting

79038. Cardenas-Jiron, G.I., J.R. Letelier and A. Toro-Labbe, "The Internal Rotation of Hydrogen Thioperoxide: Energy, Chemical Potential and Hardness Profiles," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7864-7871 (1998).

Isomerization
*cis,trans* HSOH
Barrier
Calculations

79039. Swihart, M.T., and R.W. Carr, "Thermal Decomposition of Dichlorosilane Investigated by Pulsed Laser Powered Homogeneous Pyrolysis," *J. Electrochem. Soc.* 144, 4357-4361 (1997).

Unimolecular Dissociation
$SiH_2Cl_2/SF_6$
IR Laser Pyrolysis
Rate Constant
Mechanism

## 40. CHEMICAL DYNAMICS - THEORY

(See also Section 37 for Photodissociation Dynamics)

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Reaction Dynamics
$M^* + H_2 / M + H_2(v,J)$
$M^* + H_2 / MH + H$
Conical Intersections
Probabilities
4 Methods Tested

79041. Chabinyc, M.L., S.L. Craig, C.K. Regan and J.I. Brauman, "Gas Phase Ionic Reactions: Dynamics and Mechanism of Nucleophilic Displacements," *Science* 279, 1882-1886 (1998).

Reaction Dynamics
$X^- + RY / RX + Y^-$
Rate Theory
Gas/Solution
Overview

79042. Guadagnini, R., G.C. Schatz and S.P. Walch, "Ab Initio and RRKM Studies of the Reactions of C, CH and $^1CH_2$ with Acetylene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5857-5866 (1998).

Reaction Dynamics
$C, CH + C_2H_2$
$^1CH_2 + C_2H_2$
RRKM Theory
Rate Constants
Intermediates
Lifetimes

79043. Korchowiec, J., and T. Uchimaru, "Mechanism of Addition of Fluoromethyl Radicals to Fluoroethylenes," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6682-6689 (1998).

Reaction Dynamics
$CH_nF_{3-n} + C_2H_mF_{4-m}$
$CH_3 + C_2H_4$
Radical/ Fluoroethylenes
Activation Energies
Mechanisms

79044. Wang, Z.-X., and M.-B. Huang, "Insertion of Methylidyne into the C-H Bond of Ethylene," *Chem. Phys. Lett.* 291, 381-386 (1998).

Reaction Dynamics
$CH + C_2H_4$
Insertion Channel
Energy Barrier

79045. Qi, J., and J.M. Bowman, "Quantum Calculations of Inelastic and Dissociative Scattering of HCO by Ar," *J. Chem. Phys.* 109, 1734-1742 (1998).

Reaction Dynamics
HCO + Ar
P.E. Surface
Cross Sections
Elastic,Inelastic
Dissociative
Channels

79046. Berry, R.J., and P. Marshall, "A Computational Study of the Reaction Kinetics of Methyl Radicals with Trifluorohalomethanes," *Int. J. Chem. Kinet.* 30, 179-184 (1998).

Reaction Dynamics
$CH_3 + CF_3X$
X=F,Cl,Br,I
Transition States
Rate Constants

79047. Jursic, B.S., "Density Functional Theory Computational Study of the Four-Centered Elimination $CH_2OH^+ \rightarrow CHO^+ + H_2$ Reaction," *J. Mol. Struct.* 425, 193-199 (1998).

Reaction Dynamics
$CH_2OH^+/CHO^+ + H_2$
Energy Barrier
Concerted Nature
DFT Method
Comparisons

79048. Sumathi, R., and M.T. Nguyen, "A Theoretical Study of the $CH_2N$ system: Reactions in Both Lowest Lying Doublet and Quartet States," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 8013-8020 (1998).

Reaction Dynamics
$CN + H_2$
$HCN + H$
$HNC + H$
$^{2,4}$P.E. Surfaces
Rate Constants
Barrier Heights
$\Delta H_f(CH_2N)$

79049. Rice, B.M., S.V. Pai and C.F. Chabalowski, "Performance of Density Functional Theory on the Potential Energy Surface of the H + OCS System," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6950-6956 (1998).

Reaction Dynamics
$OCS + H$
P.E. Surfaces
Channels
Energy Barriers
DFT Evaluations

79050. Sumathi, R., J. Peeters and M.T. Nguyen, "Theoretical Studies on the $C_2H + O_2$ Reaction: Mechanism for $HCO + CO$, $HCCO + O$ and $CH + CO_2$ Formation," *Chem. Phys. Lett.* 287, 109-118 (1998).

Reaction Dynamics
$C_2H + O_2$
Channels
Energies

79051. Cui, Q., Z. Liu and K. Morokuma, "Theoretical Study on the Mechanism of $CH_4 + C_2H_2^+$ Reaction: Mode-Enhancement Effect," *J. Chem. Phys.* 109, 56-62 (1998).

Reaction Dynamics
$C_2H_2^+ + CH_4$
Channels
$C_2H$ Bend Effects

79052. Minaev, B.F., and E.M. Kozlo, "Consideration of Spin-Orbital Coupling in Alkene Ozonolysis," *Theor. Exp. Chem., Russia* 33, 57-60 (1997).

Reaction Dynamics
$Alkene + O_3$
$^{1,3}$Surface Crossing
Role

79053. del Rio, E., R. Lopez and T.L. Sordo, "A Theoretical Study of the $H_2$ Elimination from $C_2H_5^+$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6831-6834 (1998).

Reaction Dynamics
$C_2H_5^+/C_2H_3^+ + H_2$
Energy Barrier
Mechanism

79054. Mann, D.J., and W.L. Hase, "Trajectory Studies of $S_N2$ Nucleophilic Substitution. VI. Translational Activation of the $Cl^- + CH_3Cl$ Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6208-6214 (1998).

Reaction Dynamics
$Cl^- + CH_3Cl$
Cross Sections
20-80 kcal $mol^{-1}$
Collision Energies

79055. Duncan, W.T., and T.N. Truong, "Erratum - Thermal and Vibrational State Selected Rates of the $CH_4 + Cl \leftrightarrow HCl + CH_3$ Reaction [*J. Chem. Phys.* 103, 9642-9652 (1995)]," *ibid.* 109, 3703 (1998).

Reaction Dynamics
$Cl + CH_4$
Rate Constants
Erratum

79056. Bolton, K., W.L. Hase, H.B. Schlegel and K. Song, "A Direct Dynamics Study of the $F+C_2H_4 \rightarrow C_2H_3F+H$ Product Energy Distributions," *Chem. Phys. Lett.* 288, 621-627 (1998).

Reaction Dynamics
$F+C_2H_4$
Product Energy Distributions
Calculations

79057. Honvault, P., and J.-M. Launay, "Quantum Mechanical Study of the $F+D_2 \rightarrow DF+D$ Reaction," *Chem. Phys. Lett.* 287, 270-274 (1998).

Reaction Dynamics
$F+D_2(v=0,J=0\text{-}2)$
DF(v,J) Product Distributions

79058. Aquilanti, V., S. Cavalli, D. De Fazio, A. Volpi, A. Aguilar, X. Gimenez and J.M. Lucas, "Hyperquantization Algorithm. II. Implementation for the $F+H_2$ Reaction Dynamics Including Open-Shell and Spin-Orbit Interactions," *J. Chem. Phys.* 109, 3805-3818 (1998).

Reaction Dynamics
$F(^2P_{1/2,3/2})+H_2$
Scattering
Hyperquantization Algorithm

79059. Azriel, V.M., L.Yu. Rusin, M.B. Sevryuk and J.P. Toennies, "Effect of the Angular Dependence of the Barrier Height on the Features of the $F+H_2$ Reaction," *Chem. Phys.* 232, 307-320 (1998).

Reaction Dynamics
$F+H_2$
Angular Dependence
Effects

79060. Takayanagi, T., and Y. Kurosaki, "Tunneling in the $F+H_2$ Reaction and Its Isotopic Variants: The Effect of the van der Waals Potential," *Chem. Phys. Lett.* 286, 35-39 (1998).

Reaction Dynamics
$F+H_2,HD,D_2$
Probabilities
van der Waals Effects

79061. Balakrishnan, N., V. Kharchenko, R.C. Forrey and A. Dalgarno, "Complex Scattering Lengths in Multichannel Atom-Molecule Collisions," *Chem. Phys. Lett.* 280, 5-9 (1997).

Reaction Dynamics
$H+H_2(v)$
Elastic/ Inelastic
Cross Sections
Complex Scattering Length Concept

79062. Jackle, A., and H.-D. Meyer, "Calculation of $H+H_2$ and $H+D_2$ Reaction Probabilities within the Multiconfiguration Time-Dependent Hartree Approach Employing an Adiabatic Correction Scheme," *J. Chem. Phys.* 109, 2614-2623 (1998).

Reaction Dynamics
$H+H_2(v=0,J=0\text{-}3)$
$H+D_2(v=0,J=0\text{-}3)$
Probabilities

79063. Mar, P.L., K.S. Werpetinski and M. Cook, "A Study of the Reaction $H+O_2 \leftrightarrow HO_2 \leftrightarrow O+OH$ at Four Levels of Density Functional Theory," *Chem. Phys. Lett.* 287, 195-201 (1998).

Reaction Dynamics
$H+O_2/O+OH$
$HO_2$ Intermediate
DFT
Paths

79064. Rodrigues, S.P.J., and A.J.C. Varandas, "Dynamics Study of the Reaction $Ar+HCN \rightarrow Ar+H+CN$, *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6266-6273 (1998).

Reaction Dynamics
HCN + Ar
P.E. Surface
Dissociation
Rate Constants

79065. Kaushik, R., and N.K. Ray, "Reactions of ROH(R=H,$CH_3$) with HNCO: A Theoretical Study," *Indian J. Chem. A* 36, 252-254 (1997).

Reaction Dynamics
$HNCO + H_2O$
$HNCO + CH_3OH$
4-Center TS
Energies
Channels

79066. Nguyen, M.T., R. Sumathi, D. Sengupta and J. Peeters, "Theoretical Analysis of Reactions Related to the $HNO_2$ Energy Surface: OH+NO and H+$NO_2$," *Chem. Phys.* 230, 1-11 (1998).

Reaction Dynamics
$HNO_2$
P.E. Surface
$H + NO_2$
OH + NO
Channels
Energies

79067. Jitariu, L.C., and D.M. Hirst, "An ab Initio Study of the Singlet Potential Energy Surface for the Reaction of $NO_3$ with $HO_2$," *J. Chem. Soc., Faraday Trans.* 94, 1379-1384 (1998).

Reaction Dynamics
$HO_2 + NO_3$
P.E. Surfaces
Energies
Channels

79068. Martin, P.G., W.J. Keogh and M.E. Mandy, "Collision Induced Dissociation of Molecular Hydrogen at Low Densities," *Astrophys. J.* 499, 793-798 (1998).

Reaction Dynamics
$H_2(0,0) + H_2$
$H_2 + H,He,e^-$
Collision Induced Dissociation
Rate Constants
1000-30000 K

79069. De, N.K., and B.R. De, "On the Mechanism of Gas Phase Decomposition of Hydrogen Peroxide: A Theoretical Study," *Indian J. Chem. A* 36, 210-212 (1997).

Reaction Dynamics
$H_2O_2$
Dissociation
P.E. Surface
Channels

79070. Clary, D.C., "Quantum Theory of Chemical Reaction Dynamics," *Science* 279, 1879-1882 (1998).

Reaction Dynamics
$H_3O^-$
$OH^-(H_2)$
Photodetachment
Transition State
Probing

79071. Clarke, N.J., M. Sironi, M. Raimondi, S. Kumar, F.A. Gianturco, E. Buonomo and D.L. Cooper, "Classical and Quantum Dynamics on the Colinear Potential Energy Surface for the Reaction of Li and $H_2$," *Chem. Phys.* 233, 9-27 (1998).

Reaction Dynamics
$Li + H_2$ /
LiH + H
P.E. Surface
Channels

79072. Voronin, A.I., J.M.C. Marques and A.J.C. Varandas, "Trajectory Surface Hopping Study of the $Li+Li_2(X^1\Sigma_g^+)$ Dissociation Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6057-6062 (1998).

Reaction Dynamics
$Li+Li_2$
Dissociation
Translational
Energy Dependences
Nonadiabatic
Contributions

79073. Baker, L.A., and S. Su, "An ab Initio Molecular Orbital Study of the Reaction $NH_2+NO \rightarrow H_2+N_2O$," *Chem. Phys.* 228, 9-16 (1998).

Reaction Dynamics
$NH_2+NO$
P.E. Surface
Channels
Energies

79074. Wang, W., R. Gonzalez-Jonte and A.J.C. Varandas, "Quasiclassical Trajectory Study of the Environmental Reaction $O+HO_2 \rightarrow OH+O_2$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6935-6941 (1998).

Reaction Dynamics
$O+HO_2$
Cross Sections
Kinetic Energy
Dependences
Rate Constants

79075. Kosmas, A.M., and E. Drougas, "Quasiclassical Trajectory Calculations of the Diatom-Diatom Reaction $OH+Cl_2 \rightarrow HOCl+Cl$ Using Two Model Potential Energy Surfaces," *Chem. Phys.* 229, 233-244 (1998).

Reaction Dynamics
$OH+Cl_2$
P.E. Surfaces
Rate Constants
Reactant
Vibrational Effects

79076. Zhang, D.H., J.C. Light and S.-Y. Lee, "Quantum Rate Constants for the $H_2+OH$ Reaction with the Centrifugal Sudden Approximation," *J. Chem. Phys.* 109, 79-86 (1998).

Reaction Dynamics
$OH+H_2$
Rate Constants
Accuracies

79077. Fast, P.L., and D.G. Truhlar, "Variational Reaction Path Algorithm," *J. Chem. Phys.* 109, 3721-3729 (1998).

Reaction Dynamics
$OH+H_2$
Path Algorithm
VTST

79078. Zhang, D.H., and S.-Y. Lee, "Effects of Reagent Rotation on the Dynamics of the $H_2+OH$ Reaction: A Full Dimension Quantum Study," *J. Chem. Phys.* 109, 2708-2716 (1998).

Reaction Dynamics
$OH+H_2$
Rate Constants
Reactant J
Effects

79079. Hand, M.R., C.F. Rodriquez, I.H. Williams and G.G. Balint-Kurti, "Theoretical Estimation of the Activation Energy for the Reaction $HO+H_2O \rightarrow H_2O+OH$: Importance of Tunneling," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5958-5966 (1998).

Reaction Dynamics
$OH+H_2O$
H-Atom Transfer
Energy Barriers
Tunneling Effects
Rate Constants

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Reaction Dynamics
$^1O_2 + R_2S$
P.E. Surfaces
Transition States
Energies

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Reaction Dynamics
$O_3/O + O_2$
$^{1,3}$Surface Crossing
Roles

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Reaction Dynamics
$Pd_3, Pt_3 + CH_4$
$Pd_3, Pt_3 + H_2$
Reactivities
Activation Energies

79083. Westerberg, J., and M.R.A. Blomberg, "Methane Activation by Naked $Rh^+$ Atoms: A Theoretical Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7303-7307 (1998).

Reaction Dynamics
$Rh^+ + CH_4$
P.E. Surface
$H_2$ Product Channel
Activation Energy
Calculations

79084. Stirling, A., "Oxygen Abstraction from $N_2O$ with Ground State Transition Metal Atoms: Density Functional Study on the Mechanism of the Reactions of Sc, Ti and $V + N_2O$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6565-6570 (1998).

Reaction Dynamics
Sc,V,Ti + $N_2O$
O-Abstraction
Mechanism

79085. Espinosa-Garcia, J., J. Sanson and J.C. Corchado, "The $SiH_4 + H \rightarrow SiH_3 + H_2$ Reaction: Potential Energy Surface, Rate Constants and Kinetic Isotope Effects," *J. Chem. Phys.* 109, 466-473 (1998).

Reaction Dynamics
$SiH_4 + H$
P.E. Surface
D Analogs
Rate Constants

## 41. CHEMICAL KINETICS - GENERAL

(See also Section 42 for Reaction Laser Control Methods)

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Oscillatory
Kinetics
Modeling

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Kinetic Rates
Stirred Reactors
Imperfect Mixing
Dead Zone
Effects

| | | |
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| 79088. | Nowakowski, B., "Nonequilibrium Molecular Velocity Distribution in Binary Reactive Gaseous Mixture," *J. Chem. Phys.* 109, 3443-3451 (1998). | Binary Reactions<br>Gas Phase<br>Diffusion Coefficients<br>Reaction Rates<br>Nonequilibrium<br>Velocity<br>Distribution<br>Effects |
| 79089. | Azatyan, V.V., and H.G. Wagner, "Induction Periods of Chemical Processes," *Kinet. Catal., Russia* 39, 149-157 (1998). | Accelerating<br>Chain Reactions<br>Induction Period<br>Definition<br>Kinetic Relationship |
| (78508) | Excitation, Rotational Temperatures, $e^-$ Densities, $C_2H_5OH$, $H_2$ Effects | Microwave<br>Ar,$N_2$,Air Plasmas |
| 79090. | Taylor, P.H., L. Cheng and B. Dellinger, "The Influence of Nitric Oxide on the Oxidation of Methanol and Ethanol," *Combust. Flame* 115, 561-567 (1998). | $CH_3OH/O_2$<br>$C_2H_5OH/O_2$<br>NO Additive<br>Perturbation<br>Effects |
| (78421) | $C_{2+}$ Hydrocarbons Synthesis, Fuel Upgrade, Catalyst Effects, Product Yields | $CH_4$ Discharge |
| 79091. | Motret, O., S. Pellerin, M. Nikravech, V. Massereau and J.M. Pouvesle, "Spectroscopic Characterization of $CH_4+CO_2$ Plasmas Excited by a Dielectric Barrier Discharge at Atmospheric Pressure," *Plasma Chem. Plasma Process.* 17, 393-407 (1997). | $CH_4/CO_2$<br>Plasma Discharge<br>$C_2$(d-a)<br>Rotational<br>Temperatures |
| (78943) | Microwave Discharge, Products, Kinetic Modeling | $CH_4/N_2$ |
| (78778) | $CH_2CHO$ and 5 $CH_3$-Substituted Vinoxy Radicals, LIF Spectra, Detected in the Reaction of O-Atom with Alkenes | Alkenes+O |
| (79028) | $C_2H_4.NO_2$ Initiation, $CH_2CHO$ Vinoxy Product Radical LIF, ps Pump/Probe Method | $C_2H_4+O$ |
| 79092. | Horie, O., and G.K. Moortgat, "The Effect of the Addition of CO on the Reaction of Ozone with Ethene," *Chem. Phys. Lett.* 288, 464-472 (1998). | $C_2H_4+O_3$<br>OH Formation<br>Yields<br>CO Scavenging<br>Method |
| 79093. | Neeb, P., O. Horie and G.K. Moortgat, "The Ethene/Ozone Reaction in the Gas Phase," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6778-6785 (1998). | $C_2H_4+O_3$<br>Criegee<br>Intermediate<br>Reactions<br>$^{13}C$ Labeling<br>Mechanistic Details |

79094. Kaiser, E.W., "Formation of $C_3H_6$ from the Reaction $C_3H_7+O_2$ between 450 and 550 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5903-5906 (1998).

$C_3H_7+O_2$
$C_3H_6$ Product Yields
Mechanism

79095. Bierbach, A., I. Barnes and K.H. Becker, "FTIR Product Study of the Gas Phase Br-Initiated Oxidation of *trans*-2-Butene under Atmospheric Conditions between 246 and 298 K," *Tellus B. Chem. Phys. Meteor.* 49, 566-582 (1997).

*trans*-2-$C_4H_8/O_2$
Br Initiated
Product FTIR Analysis
T,NO Effects

79096. Atkinson, R., E.C. Tuazon and S.M. Aschmann, "Products of the Gas Phase Reaction of the OH Radical with 3-Methyl-1-butene in the Presence of NO," *Int. J. Chem. Kinet.* 30, 577-587 (1998).

$C_5H_{10}$/OH/NO
Product Yields
Mechanisms

(78699) $C_6H_6$ Formation, Flow Reactor, Products

*t*-$C_4H_9OCH_3/O_2$

79097. Chai, Y., and L.D. Pfefferle, "An Experimental Study of Benzene Oxidation at Fuel-Lean and Stoichiometric Equivalence Ratio Conditions," *Fuel* 77, 313-320 (1998).

$C_6H_6/O_2$
Stirred Reactor
Products
Major Radicals

79098. de los Arcos, T., C. Domingo, V.J. Herrero, M.M Sanz, A. Schulz and I. Tanarro, "Diagnostics and Kinetic Modeling of a Hollow Cathode $N_2O$ Discharge," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6282-6291 (1998).

$N_2O$
Hollow Cathode
Discharge
Major Species
Measurements
Kinetic Modeling

## 42. LASERS/INDUCED EFFECTS/MPI

79099. Park, S.M., H. Chae, S. Wee and I. Lee, "Anomalous Enrichment of $C_2^+$ Ions by Laser Ablation of Graphite in Ar Jet," *J. Chem. Phys.* 109, 928-931 (1998).

Laser Ablation
Graphite
Ar Jet
$C^+,C_2^+,C_3^+$
Branching
$C_2^+$ Enhancements

79100. Guan, W., T. Matsumoto and T. Kawai, "Time and Space-Resolved Diagnosis of Laser Ablation Plasma Probed by Optical Transmittance," *Chem. Phys. Lett.* 291, 161-166 (1998).

Laser Ablation
Ca,Sr,Ba
Plume
Specific Heat Capacities

79101. Zheng, R., M. Campbell, K.W.D. Ledingham, W. Jia, C.T.J. Scott and R.P. Singhal, "Diagnostic Study of Laser Ablated $YBa_2Cu_3O_y$ Plumes," *Spectrochim. Acta B. At. Spectrosc.* 52, 339-352 (1997).

Laser Ablation
$YBa_2Cu_3O_y$
Atom,Molecules
Plume Velocities
Post-Ionization
Mass Analysis

| | | |
|---|---|---|
| (78862)<br>(78863)<br>(78864)<br>(78865) | Atomic Analysis Method, Detection Limits, Review | Laser Induced Breakdown Spectra |
| 79102. | Rusak, D.A., B.C. Castle, B.W. Smith and J.D. Winefordner, "Excitational, Vibrational and Rotational Temperatures in Nd:YAG and XeCl Laser Induced Plasmas," *Spectrochim. Acta B. At. Spectrosc.* 52, 1929-1935 (1997). | Laser Induced Breakdown Plasma<br>Graphite<br>CN* Rotational Vibrational<br>Fe,Pb Electronic Temperatures |
| 79103. | Castle, B.C., K. Visser, B.W. Smith and J.D. Winefordner, "Level Populations in a Laser Induced Plasma on a Lead Target," *Spectrochim. Acta B. At. Spectrosc.* 52, 1995-2009 (1997). | Laser Induced Breakdown Spectra<br>Pb Target<br>Nonequilibrium Emission Lines |
| 79104. | Mishima, K., and K. Yamashita, "A Theoretical Study on Laser Control of a Molecular Nonadiabatic Process by Ultrashort Chirped Laser Pulses," *J. Chem. Phys.* 109, 1801-1809 (1998). | Laser Control<br>Photodissociation<br>fs Chirped Pulses<br>Theory |
| 79105. | Zare, R.N., "Laser Control of Chemical Reactions," *Science* 279, 1875-1879 (1998). | Laser Control<br>$CH_3I$,MPI<br>$Rb+CH_3I$<br>Methods<br>Review |
| 79106. | Fiss, J.A., L. Zhu, K. Suto, G. He and R.J. Gordon, "Mechanism of the Coherent Control of the Photoionization and Photodissociation of HI and DI," *Chem. Phys.* 233, 335-341 (1998). | Laser Control<br>$HI+h\nu$<br>$DI+h\nu$<br>Autoionization<br>Predissociation<br>$HI^+,I^+$<br>Phase Lags |
| 79107. | Oppel, M., and G.K. Paramonov, "Ultrafast Laser Control of Vibrational Dynamics for a Two-Dimensional Model of $HONO_2$ in the Ground Electronic State: Separation of Conformers, Control of the Bond Length, Selective Preparation of the Discrete and the Continuum States," *Chem. Phys.* 232, 111-130 (1998). | Laser Control<br>$HNO_3$<br>Selective Excitation<br>Modeling |
| (79209) | IPS, Measurements | Am,Cm,Bk,Cf<br>Th,Np,Pu<br>REMPI |
| (78859) | Monitor for BrO and for $Br_2$ (by $O+Br_2$ Reaction) | BrO,REMPI |
| (79004) | IR MPA/MPI, Autoionization Rates, Electronically Excited State Roles | $C_{60}$ |
| (79015) | REMPI/TOF, $CF_2I_2+h\nu$, Photofragment Monitoring, Branching Ratios, Channels | $I(^2P_{1/2,3/2})$ |

(78822) (2+1) Mode, 8 Electronic Band Systems, Assignments, IP — $SF_2$, REMPI

(78827) Rydberg States, PES Spectrum, Assignments, Constants — $Xe_2$ ,REMPI/TOF

## 43. P.E. CURVES/SURFACES/ENERGY LEVELS

(See also Section 26 for Spectral Aspects, Section 40 for Surface Dynamics)

79108. Wolniewicz, L., "Relativistic Corrections to the Energies of the EF, GK and HH $^1\Sigma_g$ States of the Hydrogen Molecule," *J. Chem. Phys.* 109, 2254-2256 (1998).

Energy Levels
$H_2$(EF,GK,HH)
Calculations

79109. Koput, J., S. Carter and N.C. Handy, "Potential Energy Surface and Vibrational-Rotational Energy Levels of Hydrogen Peroxide," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6325-6330 (1998).

v,J Energy Levels
$H_2O_2$
P.E. Surface
Calculations

79110. Salzgeber, R.F., V. Mandelshtam, C. Schlier and H.S. Taylor, "All the Adiabatic Bound States of $NO_2$," *J. Chem. Phys.* 109, 937-941 (1998).

Vibrational
Energy Levels
$NO_2$(X)
All Bound States
Calculations

79111. Santoro, F., "Statistical Analysis of the Computed $X^2A_1/A^2B_2$ Spectrum of $NO_2$: Some Insights into the Causes of Its Irregularity," *J. Chem. Phys.* 109, 1824-1832 (1998).

$NO_2$(A/X)
Interactions
Energy Level
Analysis
Irregularities

79112. Burcl, R., R.V. Krems, A.A. Buchachenko, M.M. Szczesniak, G. Chalasinski and S.M. Cybulski, "Rg+Cl($^2$P) (Rg=He,Ne,Ar) Interactions: Ab Initio Potentials and Collision Properties," *J. Chem. Phys.* 109, 2144-2154 (1998).

P.E. Curves
RgCl(A,X)
Rg=He,Ne,Ar
Well Depths
Cl($^2P_{1/2}$)+Rg
Quenching
Cross Sections
Diffusion
Coefficients

79113. Surkus, A., "Reduction of Spectra to Parameters of an Effective Diatomic Hamiltonian Containing the Generalized Potential Energy Function with Correct Long Range Part: Application to $ArH^+$ in the Ground Electronic State," *Chem. Phys. Lett.* 279, 236-240 (1997).

P.E. Curve
$ArH^+$
IR,Microwave
Inverse Spectral
Reduction
Method

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| 79114. | Ornellas, F.R., and S. Iwata, "A Theoretical Study of the Electronic Structure and Spectroscopic Properties of the Low-lying Electronic States of the Molecule AlSi," *Chem. Phys.* 232, 95-109 (1998). | P.E. Curves<br>AlSi<br>Low-lying States<br>Spectral Constants<br>Energies,D<br>Transition Probabilities<br>Lifetimes |
| 79115. | Schmidt, T.W., G.B. Bacskay and S.H. Kable, "Ab Initio Potential Energy Surface and Vibrational Frequencies of HCF($A^1A''$)," *Chem. Phys. Lett.* 292, 80-86 (1998). | P.E. Surface<br>CHF($A^1A''$)<br>Spectral Constants<br>Frequencies<br>Geometry<br>Calculations |
| (79142) | P.E. Surfaces, Isomers, Geometries, Energies, Structural Calculations | $CH_2Cl_2$ ,$CH_2Cl_2^+$ |
| (78606) | P.E. Surface, Radiative Recombination, Rate Constants | $CH_3^+ + H_2$ |
| (79182) | P.E. Surface, IVR, SEP Spectra, Measurements | $CSCl_2$ |
| 79116. | Peric, M., B. Ostojic and B. Engels, "Ab Initio Study of the Electronic Spectrum of $C_2H_2^+$: Investigation of Structure of Spectra Involving Low-lying Doublet Electronic States," *J. Chem. Phys.* 109, 3086-3095 (1998). | P.E. Surfaces<br>$C_2H_2^+$(B,A,X)<br>Low-lying States<br>Frequencies<br>Energies |
| 79117. | Wang, Y.-G., C.-J. Sun and C.-H. Deng, "A Theoretical Study of $C_2H_3ONa$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5816-5821 (1998). | P.E. Surface<br>$C_2H_3ONa$<br>Isomers<br>Energy Barriers |
| 79118. | Naumkin, F.Y., and F.R.W. McCourt, "On the Influence of Rare Gas Atom/Chlorine Ion Potentials on the Ground State Rg-$Cl_2$ Interactions," *Chem. Phys. Lett.* 292, 63-70 (1998). | P.E. Curves<br>$Cl_2$.He;$Cl_2$.Ne<br>$Cl_2$.Ar<br>Ion Pair State Effects |
| 79119. | Prudente, F.V., and J.J.S. Neto, "The Fitting of Potential Energy Surfaces Using Neural Networks: Application to the Study of the Photodissociation Processes," *Chem. Phys. Lett.* 287, 585-589 (1998). | P.E. Surfaces<br>$HCl^+ + h\nu$<br>Fitting Process<br>Cross Section<br>Calculations |
| 79120. | Skokov, S., K.A. Peterson and J.M. Bowman, "An Accurate ab Initio HOCl Potential Energy Surface, Vibrational and Rotational Calculations and Comparison with Experiment," *J. Chem. Phys.* 109, 2662-2671 (1998). | P.E. Surface<br>HOCl<br>v,J Levels<br>Spectral Data<br>Comparisons |

79121. Minaev, B.F., and H. Agren, "Response Theory Calculations of the Singlet-Triplet Transition Probabilities in the HOCl Molecule," *J. Chem. Soc., Faraday Trans.* 94, 2061-2067 (1998).

P.E. Surfaces
$HOCl(^3A',^3A'',X^1A^1)$
$^{1,3}$Transition Probabilities

(79037) P.E. Surface Fitting, Isomerization

$HOO^-/OOH^-$

79122. Garcia, V.M., R. Caballol and J.P. Malrieu, "Treatment of Core-Valence Correlation Effects through Difference-Dedicated Configuration Interaction: Application to the Lowest Electronic States of K, Rb, KH, RbH and $K_2$," *J. Chem. Phys.* 109, 504-511 (1998).

P.E. Curves
$KH,K_2,RbH$
Low-lying States
Spectral Constants
$D_e,T_e$

79123. Aquilanti, V., D. Ascenzi, D. Cappelletti, M. de Castro and F. Pirani, "Scattering of Aligned Molecules: The Potential Energy Surfaces for the Kr-$O_2$ and Xe-$O_2$ Systems," *J. Chem. Phys.* 109, 3898-3910 (1998).

P.E. Surfaces
$KrO_2,XeO_2$
Scattering
Cross Section
Measurements
Well Depths

79124. Urbanski, K., S. Antonova, A.M. Lyyra, L. Li and B. Ji, "The $G^1\Pi_g$ State of $^7Li_2$ Revisited: Observation and Analysis of High Vibrational Levels," *J. Chem. Phys.* 109, 912-918 (1998).

P.E. Curve
$Li_2(G)$
OODR Spectra
v=20-48,J=1-25
Measurements

79125. Ivanov, V.S., and V.B. Sovkov, "Determination of the Potential Curve of the Bound State of a Diatomic Molecule by the WKB Method from the Spectrum of the Bound-Free Electronic Transition from the Selectively Populated Rovibronic Level," *Opt. Spectrosc., Russia* 83, 834-836 (1997).

P.E. Curves
$Li_2(^3\Pi_g$-a)
Bound-Free Spectral
Inversion Method

79126. Tan, H., M. Liao, D. Dai and K. Balasubramanian, "Potential Energy Surfaces for Mo+CO and W+CO," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6801-6806 (1998).

P.E. Surfaces
MoCO,WCO
Low-lying States
Spectral Constants
$D_e,T_e$
Calculations

79127. Stallcop, J.R., and H. Partridge, "The $N_2$-$N_2$ Potential Energy Surface," *Chem. Phys. Lett.* 281, 212-220 (1997).

P.E. Surface
$(N_2)_2$
Calculations

79128. Tan, H., D. Dai and K. Balasubramanian, "Spectroscopic Properties and Potential Energy Curves for Fifteen Electronic States of Palladium Carbide, PdC," *Chem. Phys. Lett.* 286, 375-381 (1998).

P.E. Curves
PdC
Low-lying States
Spectral Constants

79129. Ornellas, F.R., and A.C. Borin, "A Theoretical Characterization of the Quartet States of the $SO^+$ Molecular Ion," *J. Chem. Phys.* 109, 2202-2209 (1998).

P.E. Curves
$SO^+$
Low-lying
Quartet States
Spectral Constants
F.C. Factors
A-Coefficients

(78626) P.E. Surface, Rate Constant, Energy Barrier, Measurements

$SO_2^+ + H_2$

79130. Daoudi, A., S. Elkhattabi, G. Berthier and J.P. Flament, "On the Electronic Structure and Spectroscopy of the ScN Molecule," *Chem. Phys.* 230, 31-44 (1998).

P.E. Curves
ScN
Low-lying States
Spectral Constants
Bonding

79131. Kalemos, A., and A. Mavridis, "Bonding Investigation of the Ground and Low-lying States of the Titanium Boride Cation, $TiB^+$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5982-5992 (1998).

P.E. Curves
$TiB^+$
Low-lying States
Spectral Constants
$D_e$,Energies

## 44. ATOMIC/MOLECULAR STRUCTURES

(See also Section 26 for Spectrally Measured Structures)

79132. Bagatur'yants, A.A., A.A. Safonov, H. Stoll and H.-J. Werner, "Ab Initio Relativistic Pseudopotential Study of Small Silver and Gold Sulfide Clusters $(M_2S)_n$, n=1 and 2," *J. Chem. Phys.* 109, 3096-3107 (1998).

Structural
Calculations
$Ag_2S$,$Au_2S$
$(Ag_2S)_2$,$(Au_2S)_2$
Geometries
Dipole Moments
D

79133. Yang, H., K. Tanaka and M. Shinada, "On the Equilibrium Structure of $MgC_2$ and $AlC_2$," *J. Mol. Struct.* 422, 159-165 (1998).

Structural
Calculations
$AlC_2$,$MgC_2$
Geometries

79134. Berthomieu, D., Y. Bacquet, L. Pedocchi and A. Goursot, "Trimethylaluminum Dimer Structure and Its Monomer Radical Cation: A Density Functional Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7821-7827 (1998).

Structural
Calculations
$Al(CH_3)_3$
$Al(CH_3)_3^+$
$(Al(CH_3)_3)_2$
Geometries
Frequencies
D,IP

79135. Archibong, E.F., and A. St-Amant, "Molecular Structure of the $AlO_2$ Dimer, $Al_2O_4$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6877-6882 (1998).

Structural
Calculations
$Al_2O_4$
Geometry
Frequencies
IR Intensities
$D_e$

79136. Baeck, K.K., and R.J. Bartlett, "Ab Initio Study for the Low-lying Electronic States of $Al_3$ and $Al_3^-$: The Photoelectron Spectroscopy of $Al_3^-$," *J. Chem. Phys.* 109, 1334-1342 (1998).

Structural
Calculations
$Al_3$,$Al_3^-$
Low-lying States
Geometries
Frequencies
Photoelectron
Spectral Interpretation

79137. Parthiban, S., and T.J. Lee, "Ab Initio Investigation of the Atmospheric Molecule Bromine Nitrate: Equilibrium Structure, Vibrational Spectrum and Heat of Formation," *J. Chem. Phys.* 109, 525-530 (1998).

Structural
Calculations
$BrONO_2$
Geometry
Frequencies
IR Intensities
$\Delta H_f$

79138. Guha, S., and J.S. Francisco, "A Density Functional Study of the Equilibrium Structure, Vibrational Spectrum and Heat of Formation of $Br_2O_3$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6702-6705 (1998).

Structural
Calculations
$Br_2O_3$
Geometry
Frequencies
$\Delta H_f$

79139. Schuster, P., H. Mikosch and G. Bauer, "All Electron Density Functional Study of Neutral and Ionic Polybromine Clusters," *J. Chem. Phys.* 109, 1833-1844 (1998).

Structural
Calculations
$Br_3$,$Br_4$,$Br_5$
$Br_3^{\pm}$,$Br_4^{\pm}$,$Br_5^{\pm}$
Geometries
Frequencies
D,IP,EAS

79140. Li, Z., and J.S. Francisco, "High Level ab Initio Molecular Orbital Study of the Structures and Vibrational Spectra of $CHBr^+$ and $CBr^+$," *J. Chem. Phys.* 109, 134-138 (1998).

Structural
Calculations
$CBr^+$,$CHBr^+$
CBr,CHBr
Geometries
Frequencies
IPS

79141. Paddison, S.J., and E. Tschuikow-Roux, "Structures, Vibrational Frequencies, Thermodynamic Properties and Bond Dissociation Energies of the Bromomethanes and Bromomethyl Radicals: an ab Initio Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6191-6199 (1998).

Structural Calculations
$CH_{4-n}Br_n$
$CH_{3-m}Br_m$
Geometries
Frequencies
$\Delta H_f$ ,$\Delta G$,$K_p$
0-1500 K Values

79142. Lewars, E., "The Isomers of Dichloromethane and Its Radical Cation: an ab Initio Exploration of the Neutral and Charged $CH_2Cl_2$ Potential Energy Surfaces," *J. Mol. Struct.* 425, 207-226 (1998).

Structural Calculations
$CH_2Cl_2$ ,$CH_2Cl_2^+$
Isomers
Geometries
Energies
P.E. Surfaces

79143. Gellene, G.I., "$CO_2^+$: A Difficult Molecule for Electron Correlation," *Chem. Phys. Lett.* 287, 315-319 (1998).

Structural Calculations
$CO_2^+$
Geometry
Theoretical Difficulties

79144. Yamaguchi, Y., J.C. Rienstra-Kiracofe, J.C. Stephens and H.F. Schaefer III, "The Hydroxyethynyl Radical (CCOH): An Accessible Isomer of the Ketenyl Radical (HCCO)?," *Chem. Phys. Lett.* 291, 509-516 (1998).

Structural Calculations
CCOH(A,X)
Geometries
Energies
IR Intensities

79145. Bauer, S.H., and C.F. Wilcox, "On Malonaldehyde and Acetylacetone: Are Theory and Experiment Compatible?," *Chem. Phys. Lett.* 279, 122-128 (1997).

Structural Calculations
$CH_2(CHO)_2$
$CH_2(COCH_3)_2$
Spectral Data
Discrepancies
Isomeric Forms
Stabilities

79146. Politzer, P., J.S. Murray and M.C. Concha, "C-H and C-$NO_2$ Dissociation Energies in Some Azines and Nitroazines," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6697-6701 (1998).

Structural Calculations
Aromatic Azines
Nitroazines
Benzene Ring
Nitrogens
D(C-H,C-$NO_2$)
20 Molecules

79147. Han, Y.-K., Y.S. Lee, S.Y. Lee and J.T. Kim, "Ab Initio Study of Fluorocyclobutenes: An Attempt to Resolve the Difference between Microwave Spectroscopy and Electron Diffraction Geometries of Hexafluorocyclobutene," *J. Mol. Struct.* 422, 25-33 (1998).

Structural
Calculations
*c*-$C_4F_6$ ,*c*-$C_4H_6$
*c*-$C_4H_4F_2$ ,*c*-$C_4H_2F_4$
*c*-$C_4Cl_2F_4$
Geometries
Microwave/
Electron Diffraction
Disagreements

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Structural
Calculations
$C_4H_4$
$^{1,3}$Splitting
Geometry
Frequencies
Self-Polymerization

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Structural
Calculations
*c*-$C_4H_4N_2$ ,$C_6H_6$
Geometries
Frequencies
Vibronic Structure

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Structural
Calculations
$CH_2CHCHCH$
Isomers
Geometries
Frequencies
Energies
Isomerizations

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Structural
Calculations
$C_{10}H_8$ ,$C_{10}H_8^+$
$CHO,CH_2OH,OH,O$
Group Substitution
Effects
Frequencies
IR Intensities

79152. Bauschlicher Jr, C.W., "Infrared Spectra of Polycyclic Aromatic Hydrocarbons: Nitrogen Substitution," *Chem. Phys.* 234, 87-94 (1998).

Structural
Calculations
$C_{10}H_8$ ,$C_{14}H_{10}$
$N,CN,NH,NH_2$
Group Substitution
Effects
IR Frequencies
Relative Intensities

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Structural
Calculations
$C_{10}H_7CH_3$
$C_{14}H_9CH_3$
Neutrals/Cations
Isomers
Frequencies
IR Intensities
H Loss Effects

79154. Workman, M.A., and J.S. Francisco, "Molecular Structure and Energetics of *sym*-$ClO_3$," *Chem. Phys. Lett.* 279, 158-164 (1997).

Structural
Calculations
*sym*-$ClO_3$
Geometry
Frequencies
$\Delta H_f$

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Structural
Calculations
CuX,AgX,AuX
(X=H,F,Cl)
$Cu_2$,$Ag_2$,$Au_2$
CuAg,CuAu,AgAu
Spectral Constants
$D_e$

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Structural
Calculations
$F_3^+$,$Cl_3^+$
Low-lying States
Geometries
Frequencies
Stabilities

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Structural
Calculations
GeH,$GeCH_3$
$GeC_2H_5$
Geometries
Frequencies

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Structural
Calculations
$Ge_n$,$Ge_n^-$
n=2-6
Geometries
Frequencies
EAS

79159. Schutz, M., G. Rauhut and H.-J. Werner, "Local Treatment of Electron Correlation in Molecular Clusters: Structures and Stabilities of $(H_2O)_n$, n=2-4," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 5997-6003 (1998).

Structural
Calculations
$(H_2O)_n$,n=2-4
Geometries
Stabilities

79160. Adamo, C., and P. Maldivi, "A Theoretical Study of Bonding in Lanthanide Trihalides by Density Functional Methods," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6812-6820 (1998).

Structural
Calculations
$LaX_3$,$GdX_3$
$LuX_3$
X=F,Cl,Br,I
Geometries
Frequencies
Atomization
Energies

79161. Kieninger, M., K. Irving, F. Rivas-Silva, A. Palma and O.N. Ventura, "Density Functional and ab Initio Study of the Free Radical MgNC," *J. Mol. Struct.* 422, 133-141 (1998).

Structural
Calculations
MgNC
Geometry
Spectral Constants

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Structural
Calculations
$NO.^+Rg$
Rg=He,Ne,Ar,Kr,Xe
Geometries
Frequencies
Energies

79163. Shen, Q., and K. Hedberg, "Investigation of the Equilibrium $N_2O_4 \leftrightarrow 2NO_2$ by Electron Diffraction: Molecular Structures and Effective Temperature and Pressure of the Expanding Gas with Implications for Studies of Other Dimer-Monomer Equilibria," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6470-6476 (1998).

Structures
$NO_2$,$N_2O_4$
Nozzle Jet
T,P Dependences
Electron
Diffraction

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Structural
Calculations
$(NO)_2$
Low-lying
Electronic States
Energies
Assignments

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Structural
Calculations
$Nb_n$,$Mo_n/N_2$
n=1-4
Geometries
Frequencies
Electronic States
D,IP(MoN,NbN)

79166. Barysz, M., and M.G. Papadopoulos, "On the Ground State of $NiH_2$," *J. Chem. Phys.* 109, 3699-3700 (1998).

Structural
Calculations
$NiH_2$
Geometry
Dipole Moment
$(X^1A_1)$ Bent State

(78624) Structural Calculations, n=1-3, Geometries, EAS — $PCl_n$, $POCl_n$ $PCl_n^-$, $POCl_n^-$

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79169. Nayak, S.K., B.K. Rao, S.N. Khanna and P. Jena, "Atomic and Electronic Structure of Neutral and Charged $Si_nO_m$ Clusters," *J. Chem. Phys.* 109, 1245-1250 (1998). — Structural Calculations $Si_nO_m$ $n \leq 6, m \leq 12$ Geometries D, IP, EAS

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## 45. ENERGY TRANSFER

(See also Section 27 for Electronically Excited State Relaxation Processes)

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(78807) Rydberg States, E-E Relaxation, ASE Decay, (T-R), (Z-Y) Nearby States, Term Values

NO(T,$Z^2\Sigma^+$)

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E-E Transfer
NO(B/a)
Gateway States
Magnetic Field Effects

79175. Bae, S.C., H.S. Yoo and J.K. Ku, "Intersystem Crossing Rate Constants from the (0,4,1) and (1,2,1) Levels of the $A^1A_2$ to $a^3B_1$ State of $SO_2$," *J. Chem. Phys.* 109, 1251-1258 (1998).

E-E Transfer
$SO_2$(A/a)
v,J Relaxation
$SO_2$(A)
Lifetimes
Rate Constants

79176. Breckenridge, W.H., M.D. Morse and J.G. McCaffrey, "A Pair Potentials Study of Matrix-isolated Atomic Zinc. II. Intersystem Crossing in Rare Gas Clusters and Matrices," *J. Chem. Phys.* 109, 3137-3144 (1998).

E-E Transfer
Zn($^1P_1$/ $^3P_J$)/Rg
Intersystem Crossing
Matrix Study

79177. Calasso, I.G., I. Delgadillo and M.W. Sigrist, "Modeling and Analysis of Experimental Photothermal Beam Deflection Signals in Gases," *Chem. Phys.* 229, 181-191 (1998).

Energy Relaxation
Optothermal
Beam Deflection
New Model
Decay Rates

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IVR
Molecular
Energy Flow
Review

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IVR
Polyatomics
fs Pump/Probe
Proposed Method

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V-V Transfer
CO(v=1)+$CD_3H$
Rate Constants
$H_2$,He,Ne
Buffer Gas
Collision Effects
70-100 K

79181. Millot, G., and C. Roche, "State-to-State Vibrational and Rotational Energy Transfer in $CO_2$ Gas from Time-Resolved Raman-Infrared Double Resonance Experiments," *J. Raman Spectrosc.* 29, 313-320 (1998).

v,J Relaxation
$CO_2$
5 Lower Vibrational Levels
Transfer Rates
J Fitting Laws

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IVR
$CSCl_2$
SEP Spectra
P.E. Surface

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Vibrational Relaxation
$CClF_2CHCl_2(v) + M$
Rates
IR MPD
Comparisons

79184. Henton, S., M. Islam and I.W.M. Smith, "Intramolecular V-V Transfer between the Components of the $(3_1/2_14_15_1)$ and $(3_14_1/2_14_25_1)$ Fermi Dyads in Acetylene in $C_2H_2/C_2H_2$ Collisions," *Chem. Phys. Lett.* 291, 223-230 (1998).

V-V Transfer
$C_2H_2/C_2H_2$
Intradyad
Rate Constant
Measurements

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IVR
$C_2H_2(X)$
$v = 10000\text{-}15000\ cm^{-1}$
Slow Relaxation
(A-X) LIF Probe

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Vibrational Energy Transfer
*c*-$C_4H_4N_2$
Conical Intersection
Model

(79032) Vibrational Relaxation Rate Constants, Unimolecular Dissociation, Shock Tube

*c*-$C_4H_4O$ + Ne,Kr

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Vibrational Relaxation
$C_6F_6(v)$
IRMPA
(14500-17500 $cm^{-1}$)
UV Pumping
(40300 $cm^{-1}$)
Direct Comparisons
Agreement

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IVR
$C_6H_6(3\nu_{CH})$
Vibrational
Level Mixing
Calculations

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Vibrational
Average
Energy Transfers
$C_6H_5CH_2(v) + M$
$M = He, Ar, N_2$
$C_3H_8, C_7H_{16}, C_8H_{18}$

79190. Heidelbach, C., J. Schroeder, D. Schwarzer and V.S. Vikhrenko, "Mode Specificity of Vibrational Energy Relaxation of Azulene in $CO_2$ at Low and High Density," *Chem. Phys. Lett.* 291, 333-340 (1998).

Vibrational
Relaxation
*c*-$C_{10}H_8/CO_2$
Density Effects
Calculations

(79034) Energy Flow, Molecular Isomerization, Model

*trans/cis*$(C_6H_5CH)_2$

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Vibrational
Relaxation
$C_{70}(v) + He, Ar$
Efficiencies
Calculations

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Vibrational
Relaxation
$HCl(v=1) + M$
Rate Constants
$M = HCl/CO_2/(Ar)$
LIF Monitor

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Vibrational
Relaxation
$H_2(v) + H$
Rate Constants
Low Temperatures
Calculations

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Vibrational
Relaxation
$H_2(v) + He$
Cross Sections
Low Temperatures
$H_2(v)$.He Lifetime

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V-V Transfer
$NO(v) + N_2O$
v=20-22
Energy Defects
Rotational Role

(78619) Vibrational Relaxation/Reactive Rate Constants, Branching Ratios

$N_2^+(v=0\text{-}3) + HCl$

79196. Reid, J.P., P.W. Barnes and C.J.S.M. Simpson, "The Vibrational Deactivation of $N_2(v=1)$ by $H_2$ and HD at Low Temperatures," *Chem. Phys. Lett.* 280, 359-366 (1997).

Vibrational Relaxation
$N_2(v=1)+H_2,HD$
Rate Constants
55-200 K
$N_2$ Isotope Effects

79197. Kato, S., V.M. Bierbaum and S.R. Leone, "Multiquantum Vibrational Deactivation of $N_2^+(v)$ by Collisions with $N_2$ and $O_2$ at Thermal Energies," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 6659-6667 (1998).

Vibrational Relaxation
$N_2^+(v)+N_2,O_2$
v=0-4
Charge Transfer
Rate Constants
Multiquantum Channels

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V-V Transfer
$N_2O(\nu_3)+C_6H_6$
$N_2O(\nu_3)+C_6D_6$
Rates
Calculations

79199. Balakrishnan, N., A. Dalgarno and G.D. Billing, "Multiquantum Vibrational Transitions in $O_2(v\geq25)+O_2(v=0)$ Collisions," *Chem. Phys. Lett.* 288, 657-662 (1998).

Vibrational Relaxation
$O_2(v\geq25)+O_2$
Multiquantum Contributions
Dominant Physical Channel

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Rotational Energy Transfer
$H+H_2$
70-1000 K
Rate Constants
Calculations

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Rotational Relaxation
HBr(J)+Ar
Free Jet
Rate Constants

79202. Flower, D.R., "The Rotational Excitation of $H_2$ by $H_2$," *Mon. Not. Roy. Astron. Soc.* 297, 334-336 (1998).

Rotational Energy Transfer
$H_2(J)+H_2(J')$
Rate Constants
200-1000 K
Calculations

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Rotational Energy Transfer
NO($X^2\Pi_{1/2}$,v=3,J)
He,Ar,$N_2$ Partners
Cross Sections
Low Temperatures
Propensities

79204. van Beek, M.C., K. Schreel and J.J. ter Meulen, "Rotational Excitation of OH in Collisions with CO, $N_2$ and $CO_2$," *J. Chem. Phys.* 109, 1302-1309 (1998).

Rotational Energy Transfer
OH+CO,$CO_2$,$N_2$
State-to-State
Cross Sections
Propensities

## 46. THERMOCHEMISTRY

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Equilibrium Compositions
Combustion Products
Simple Procedure

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$\Delta H_{Combustion}$
Solids
DSC Method
Accuracies

79207. Curtiss, L.A., P.C. Redfern, K. Raghavachari and J.A. Pople, "Assessment of Gaussian-2 and Density Functional Theories for the Computation of Ionization Potentials and Electron Affinities," *J. Chem. Phys.* 109, 42-55 (1998).

IP,EA
146 Molecules
Gaussian-2,DFT
Methods
Accuracies

(79112) Rg=He,Ne,Ar, P.E. Curves

D(RgCl(A,X))

(79132) Structural Calculations, Geometries, Dipole Moments

D($Ag_2S$,$Au_2S$)
D($(Ag_2S)_2$,$(Au_2S)_2$)

(79134) Structural Calculations, Geometries, Frequencies

D,IP($Al(CH_3)_3$)
D,IP($(Al(CH_3)_3)_2$)

(79114) P.E. Curves, Low-lying States, Spectral Constants, Energies, Transition Probabilities, Lifetimes

D(AlSi)

79208. Petrie, S., "Thermochemistry of Aluminum Halides: A Theoretical Appraisal," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7828-7834 (1998).

$D_0$,$\Delta H_f$
$AlX$,$AlX_2$,$AlX_3$
Neutrals,Ions
Mixed Halides
X=F,Cl,Br
Calculations

| | | |
|---|---|---|
| (79135) | Structural Calculations, Geometry, Frequencies, IR Intensities | $D_e(Al_2O_4)$ |
| 79209. | Kohler, S., R. Deissenberger, K. Eberhardt, N. Erdmann, G. Herrmann, G. Huber, J.V. Kratz, M. Nunnemann, G. Passler, P.M. Rao, J. Riegel, N. Trautmann and K. Wendt, "Determination of the First Ionization Potential of Actinide Elements by Resonance Ionization Mass Spectroscopy," *Spectrochim. Acta B. At. Spectrosc.* 52, 717-726 (1997). | IP<br>Am,Cm,Bk,Cf<br>Th,Np,Pu<br>REMPI Method |
| (78764) | Photoelectron Spectra, State Assignments, Spectral Constants | IP(ArKr) |
| 79210. | Feller, D., D.A. Dixon and K.A. Peterson, "Heats of Formation of Simple Boron Compounds," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7053-7059 (1998). | $\Delta H_f(BH,BH_2)$<br>$\Delta H_f(BH_3,B_2H_6)$<br>Calculations |
| (79137) | Structural Calculations, Geometry, Frequencies, IR Intensities | $\Delta H_f(BrONO_2)$ |
| (79138) | Structural Calculations, Geometry, Frequencies | $\Delta H_f(Br_2O_3)$ |
| (79139) | Structural Calculations, Geometries, Frequencies | D,IP,EAS<br>$Br_3,Br_4,Br_5$ |
| (79140) | Structural Calculations, Geometries, Frequencies | IP(CBr,CHBr) |
| (78766) | (A-X), LIF Spectrum, P.E. Surface, Lifetimes | $\Delta H_f(CFBr)$ |
| (78937) | Rate Constants, Temperature Dependences, Equilibrium Constants, Shock Tube | $CF_3+H_2/CF_3H+H$ |
| (79141) | $\Delta H_f$, $\Delta G$, $K_p$, 0-1500 K Thermodynamic Values, Geometries, Frequencies, Structural Calculations | $CH_{4-n}Br_n$<br>$CH_{3-m}Br_m$ |
| 79211. | Jursic, B.S., "C-H and C-Halogen Bond Dissociation Energies for Fluorinated and Chlorinated Methane Evaluated with Hybrid B3LYP Density Functional Theory Methods and Their Comparison with Experimental Data and the CBS-Q ab Initio Computational Approach," *J. Mol. Struct.* 422, 253-257 (1998). | $D(CH_{4-n}F_n)$<br>$D(CH_{4-n}Cl_n)$<br>n=0-4<br>Bond Energies<br>Calculations |
| (79048) | Reaction Dynamics, $CN+H_2$, $H+HCN$, $H+HNC$, $^{2,4}$P.E. Surfaces, Rate Constants, Barrier Heights, Calculations | $\Delta H_f(CH_2N)$ |
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$\Delta H_f(g)$
Nitro-Organics
Measurements
Group Additivity
Values

79215. Cheung, Y.-S., J.-C. Huang and C.Y. Ng, "Vacuum Ultraviolet Laser Pulsed Field Ionization Photoelectron Studies of Polyatomic Species: Accurate Ionization Energies of $CH_3SH$ and $CH_3CH_2SH$," *J. Chem. Phys.* 109, 1781-1786 (1998).

IP($CH_3SH$)
IP($C_2H_5SH$)
PFI-PE Spectra

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EA($CN_2$,$CHN_2$)
EA($CDN_2$)
D($CH_2N_2$)
D,$\Delta H_f$($CHN_2$)
$\Delta H_f$(HCN,$CN_2$)
Photoelectron
Spectral Measurements

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Bond Energies
$C_2H_nCl_{6-n}$
$C_2H_nCl_{5-n}$
Calculations

79218. Berry, R.J., C.J. Ehlers, D.R. Burgess Jr, M.R. Zachariah, M.R. Nyden and M. Schwartz, "Halon Thermochemistry: Ab Initio Calculations of the Enthalpies of Formation of Fluoroethanes," *J. Mol. Struct.* 422, 89-98 (1998).

$\Delta H_f(C_2H_{6-n}F_n)$
n=0-6
Calculations
Bond Additivity

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Thermodynamic
Properties
$C_2H_{6-n}F_n$
9 Molecules
Frequencies
$\Delta H_f$ $S°$ $C_p$
300-1500 K
Calculations

79220. Good, D.A., and J.S. Francisco, "Bond Dissociation Energies and Heats of Formation for Fluorinated Ethers: E143A ($CH_3OCF_3$), E134 ($CHF_2OCHF_2$), and E125 ($CF_3OCHF_2$)," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7143-7148 (1998).

$\Delta H_f$,$D_{C-H}$
$CF_3OCHF_2$
$(CHF_2)_2O$
$CF_3OCH_3$
Calculations

79221. Glukhovtsev, M.N., and R.D. Bach, "Ab Initio Study on the Thermochemistry of Vinyl Radical and Cation," *Chem. Phys. Lett.* 286, 51-55 (1998).

$\Delta H_f$ ,IP($C_2H_3$)
$\Delta H_f$(*c*-$C_2H_3^+$)
Calculations

79222. Mayer, P.M., M.S. Taylor, M.W. Wong and L. Radom, "Thermochemistry of $CH_3CN$, $CH_3NC$ and Their Cyclic Isomers and Related Radicals, Cations and Anions: Some Curious Discrepancies between Theory and Experiment," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7074-7080 (1998).

$\Delta H_f$
$CH_3CN$,$CH_3NC$
*c*-$CH_2NCH$,*c*-CH(CH)NH
$CH_2CN$,$CH_2NC$
CH(CH)N
Neutrals/Ions
Calculations
Discrepancies

79223. Seetula, J.A., "Kinetics and Thermochemistry of the $R + HBr \leftrightarrow RH + Br$ ($R = C_2H_5$ or $\beta$-$C_2H_4Cl$) Equilibrium: An ab Initio Study of the Bond Energies in Partly Chlorinated Ethanes and Propanes," *J. Chem. Soc., Faraday Trans.* 94, 891-898 (1998).

$\Delta H_f(C_2H_5, C_2H_4Cl)$
$D(C_2H_5Cl, C_3H_7Cl)$
$D(C_2H_4Cl_2)$
$C_2H_5 + HBr$
$C_2H_4Cl + HBr$
Rate Constants
T Dependences

(78781) Partition Functions, Rotational Spectrum, Constants

$(CH_3)_2O$

79224. Petrie, S., "Proton Affinities of Dicyanogen Isomers: Is there a Preferred Site of Protonation for CNCN?," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7835-7840 (1998).

$PA(C_2N_2)$
$C_2N_2$, $C_2N_2H^+$
Isomers
Isomerization
Energies
Calculations

(78955) $C_2O + M$ Unimolecular Dissociation Rate Constants, T Dependences, Shock Tube

$\Delta H_f(C_2O)$

(78934) $Br + C_3H_6 + M$ Rate Constants, Measurements

$\Delta H_f(C_3H_6Br)$

(79146) Aromatic Azines, Nitroazines, Benzene Ring Nitrogen Molecules, 20 Molecules, Structural Calculations

$D(C\text{-}H, C\text{-}NO_2)$

(78787) $X^2\Sigma^+$ Spectral Constants, Calculations

$D_0(CaAr^+, CaKr^+)$

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Cd
Molecules
Thermodynamic
Properties
Review

(78789) Laser Excitation Spectra, Constants

$D_e(CdHe(B,A,X))$

(79154) Structural Calculations, Geometry, Frequencies

$\Delta H_f(ClO_3)$

79226. Nizzi, K.E., C.A. Pommerening and L.S. Sunderlin, "Gas Phase Thermochemistry of Polyhalide Anions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7674-7679 (1998).

$D_0(Cl_3^-, Br_3^-)$
$D_0(Br_5^-)$
$EA(Cl_3, Br_3)$
Measurements

(79155) X = H,F,Cl, Spectral Constants, Structural Calculations

$D_e(CuX, AgX, AuX)$
$D_e(Cu_2, Ag_2, Au_2)$
$D_e(CuAg, CuAu, AgAu)$

| | | |
|---|---|---|
| 79227. | Duke, B.J., and L. Radom, "Gaussian-2 (G2) Theory for Third-Row Elements: A Systematic Study of the Effect of the 3*d* Orbitals," *J. Chem. Phys.* 109, 3352-3359 (1998). | D,IP<br>Ga,Ge,As<br>Se,Br,Kr<br>Molecules<br>Calculations<br>Accuracies |
| 79228. | Schmude Jr, R.W., and K.A. Gingerich, "Thermodynamic Investigation of Small Germanium-Tin Clusters with a Mass Spectrometer," *J. Chem. Phys.* 109, 3069-3071 (1998). | $D_0$(GeSn,SnC)<br>$D_0$($Ge_2Sn$,$GeSn_2$)<br>Knudsen Cell<br>Mass Analysis |
| (79158) | n=2-6, Structural Calculations, Geometries, Frequencies | EA($Ge_n$) |
| 79229. | Hansel, A., C. Scheiring, M. Glantschnig, W. Lindinger and E.E. Ferguson, "Thermochemistry of HNC, $HNC^+$ and $CF_3^+$," *J. Chem. Phys.* 109, 1748-1750 (1998). | $\Delta H_f$(HNC,$HNC^+$)<br>AP($CF_3^+/CF_4$)<br>Measurements |
| 79230. | Speranza, M., "Stable vs. Metastable HOOO: An Experimental Solution for an Evergreen Theoretical Dilemma," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7535-7536 (1998). | $\Delta H_f(HO_3)$<br>Literature<br>Assessment |
| 79231. | Braida, B., P.C. Hiberty and A. Savin, "A Systematic Failing of Current Density Functionals: Overestimation of Two-Center Three-Electron Bonding Energies," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 7872-7877 (1998). | D<br>$He_2^+$,$Ne_2^+$,$Ar_2^+$<br>$(H_2O)_2^+$,$(HCl)_2^+$,$(HF)_2^+$<br>$(H_2S)_2^+$,$(NH_3)_2^+$$(PH_3)_2^+$<br>3 Eletron Bonds<br>DFT Failures |
| (79122) | P.E. Curves, Low-lying States, Spectral Constants, $T_e$, Calculations | $D_e$(KH,$K_2$,RbH) |
| (78802) | (C-$1^1\Pi_g$) LIF Spectra, v″≤107, RKR P.E. Curve, Constants, $T_e$ | $D_e$($K_2$($1^1\Pi_g$)) |
| (79123) | P.E. Surfaces, Scattering Cross Section Measurements, Well Depths | D($KrO_2$,$XeO_2$) |
| (79160) | Atomization Energies, X=F,Cl,Br,I, Geometries, Frequencies, Structural Calculations | D($LaX_3$,$GdX_3$,$LuX_3$) |
| (78803) | Resonant Photoionization Spectrum, Constants, (F,E-X) Bands | D(LiMg) |
| (79126) | P.E. Surfaces, Low-lying States, Spectral Constants, $T_e$, Calculations | $D_e$(MoCO,WCO) |
| (79165) | Structural Calculations, Geometries, Frequencies | D,IP(MoN,NbN) |
| (78818) | PFI-PE Spectrum, $O_2^+$(c)-$O_2$(X), Constants, Linewidths, Predissociative Lifetimes | IP($O_2^+$(c,v=0,1)) |
| (78821) | $(O_2(a))_2$-$(O_2(X))_2$ Intracavity Absorption Spectra, 630, 578 nm Bands | $D_0'$,$D_0''$$(O_2)_2$ |
| (78624) | n=1-3, Structural Calculations, $PCl_3$, $POCl_3$+$e^-$ Dissociative Attachment Rate Constant Measurements | EA($PCl_n$,$POCl_n$) |
| (78822) | (2+1) REMPI Spectra, 8 Electronic Band Systems, Assignments | IP($SF_2$) |

79232. Bauschlicher Jr, C.W., and A. Ricca, "Atomization Energies of SO and $SO_2$: Basis Set Extrapolation Revisited," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 102, 8044-8050 (1998).

Atomization Energies
$SF,SF^+,SF_6$
$SO,SO_2$
Basis Set Requirements

(79169) $n \leq 6$, $m \leq 12$, Structural Calculations, Geometries

$D,IP,EAs$
$Si_nO_m$

(79131) P.E. Curves, Low-lying States, Spectral Constants, Energies

$D_e(TiB^+)$

(78826) Spectral Analysis, Constants

$D_0(VAr^+(B,X))$

## 47. EXPERIMENTAL METHODS

79233. Friedrich, B., R. deCarvalho, J. Kim, D. Patterson, J.D. Weinstein and J.M. Doyle, "Towards Magnetic Trapping of Molecules," *J. Chem. Soc., Faraday Trans.* 94, 1783-1791 (1998).

Molecular Trapping
$Eu,NO,O_2$
Potential Applications
Overview

(78847) Formation, Ultracold Photoassociation, Pumping/Decay Method

$Li_2(v,J)$

## 48. MISCELLANEOUS

## SUBJECT INDEX CATEGORIES

1. Fuels, Synfuels - General
2. Liquefaction, Gasification
3. Burners
4. Coal, Particle Combustion, Pyrolysis
5. Spray Combustion
6. Metals, Propellants, Polymer Combustion
7. Catalytic Combustion
8. MHD
9. Temperatures
10. Ignition
11. Combustion Theory, Propagation, Stabilization
12. Turbulence
13. Detonations, Explosions
14. Flow Phenomena, Velocities, Diffusion
15. Ionization
16. Inhibition, Additives
17. Corrosion, Erosion, Deposition
18. Gas, Surface Interactions, Boundary Layer Combustion
19. Engines, Emissions
20. Plume, Stack Chemistry, Atmospheric Emissions
21. Combustion Emissions, $NO_x$, $SO_2$ Chemistry, Control
22. Soot, Diamond, Particle Formation, Control
23. Particle Characterization
24. Nucleation, Coagulation, Clusters
25. Flame, Chemiluminescent Spectroscopy
26. Spectral Characterizations, Analyses
27. Excited State Lifetimes, Quenching
28. Franck-Condon Factors, Transition Probabilities
29. Lineshapes, Strengths
30. Analysis, Monitoring Techniques
31. Flame Concentration Measurements
32. Mapping, Tomographic Methods
33. Optogalvanic, Optoacoustic Methods
34. Flame Kinetic Modeling
35. Pyrolysis Kinetics, Studies
36. Kinetic Modeling, Sensitivities, Rate Constants
37. Photolysis, MPD
38. Reaction Product - Energy Distributions
39. Unimolecular Processes
40. Chemical Dynamics - Theory
41. Chemical Kinetics - General
42. Lasers, Induced Effects, MPI
43. P.E. Curves, Surfaces, Energy Levels
44. Atomic, Molecular Structures
45. Energy Transfer
46. Thermochemistry
47. Experimental Methods
48. Miscellaneous